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# Bridging the gap between SOLA and Deterministic Linear Inferences in the context of seismic tomography

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#### 5 SUMMARY

Seismic tomography is routinely used to image the Earth's interior using seismic data. How-6 ever, in practice, data limitations lead to discretised inversions or the use of regularisations, which complicates tomographic model interpretations. In contrast, Backus-Gilbert inference methods make it possible to infer properties of the true Earth, providing useful insights into 9 the internal structure of our planet. Two related branches of inference methods have been de-10 veloped - the Subtractive Optimally Localized Averages (SOLA) method and Deterministic 11 Linear Inference (DLI) approaches - each with their own advantages and limitations. In this 12 contribution, we show how the two branches can be combined to derive a new framework 13 for inference, which we refer to as SOLA-DLI. SOLA-DLI retains the advantages of both 14 branches: it enables us to interpret results through the target kernels, rather than the imperfect 15 resolving kernels, while also using the resolving kernels to inform us on trade-offs between 16 physical parameters. We therefore highlight the importance and benefits of a more careful 17 consideration of the target kernels. This also allows us to build families of models, rather than 18 just constraining properties, using these inference methods. We illustrate the advantages of 19

SOLA-DLI using three case studies, assuming error-free data at present. In the first, we illus-20 trate how properties such as different local averages and gradients can be obtained, includ-21 ing associated bounds on these properties and resolution information. Our second case study 22 shows how resolution analysis and trade-offs between physical parameters can be analysed 23 using SOLA-DLI, even when no data values or errors are available. Using our final case study, 24 we demonstrate that SOLA-DLI can be utilised to obtain bounds on the coefficients of basis 25 function expansions, which leads to discretised models with specific advantages compared to 26 classical least-squares solutions. Future work will focus on including data errors in the same 27 framework. This publication is accompanied by a SOLA-DLI software package that allows the 28 interested reader to reproduce our results and to utilise the method for their own research. 29

Key words: Inverse theory, Seismology, Seismic tomography, Structure of the Earth, Surface
 waves and free oscillations.

#### 32 1 INTRODUCTION

Seismic tomography relies on mathematical inversions (Rawlinson et al. 2010; Nolet 2008) to 33 model Earth's interior from collected data. Resulting tomography models highlight persistent fea-34 tures, such as subducted plates, rising plumes, and large scale velocity anomalies, believed to 35 mirror real Earth characteristics (Ritsema & Lekić 2020). Improving these models often involves 36 the development of new models with different data or methods to enhance the resolution of certain 37 features or to reduce uncertainties. However, seismic inversions encounter a major challenge: data 38 scarcity. This leads to non-uniqueness in solutions (e.g. Tarantola 1987), which often is mitigated 39 using regularisation. Yet, such prior information might inadvertently impose unrealistic constraints 40 or introduce artefacts in the models (e.g. Nolet 2008; Zaroli et al. 2017). While incorporating such 41 new information is not inherently wrong, it must be accurate and well-understood to avoid misin-42 terpretations of the resulting seismic tomography models. 43

In contrast, inference methods aim to constrain some specific properties of the unknown model. In geophysics, these methods can be traced back to the seminal papers of Backus and Gilbert (Backus & Gilbert 1967a,b, 1970), where they attempted to obtain the highest resolution local

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<sup>47</sup> averages of a continuous unknown model using just the data as constraints. The methodology in<sup>48</sup> troduced in Backus & Gilbert (1970) has since been used in various branches of geophysics, e.g.
<sup>49</sup> deconvolution (Oldenburg 1981), geomagnetism (Backus 1988a), seismology (Zaroli 2016). Fur<sup>50</sup> thermore, this foundational work has inspired the development of two branches of linear inference
<sup>51</sup> methods (See Fig. A1).

The first branch started with three contributions from Backus (Backus 1970a,b,c) where the 52 goal was to find a specific linear property of the unknown model, rather than just the highest res-53 olution local average. Backus showed that data alone cannot provide any information on nearly 54 all linear properties, and introduced an additional prior constraint on the model space in the form 55 of a model norm bound (Backus 1970a). The use of prior model information (e.g. a norm bound) 56 is what distinguishes this branch, which we refer to as the DLI (Deterministic Linear Inference) 57 branch due to the deterministic nature of the norm bound prior information (as opposed to a prob-58 abilistic prior information). Backus (1970b) and Backus (1970c) further investigated how to deal 59 with properties that cannot be naturally expressed on Hilbert spaces, and how to approach situa-60 tions where we have bounds on the norm of a truncated expansion of the model rather than the 61 model itself. Parker (1977) re-derived the findings of Backus (1970a) in a modified framework, 62 defining a finite-dimensional "property-data" space separate from the infinite-dimensional model 63 space. This approach was then used to constrain the coefficients of a basis expansion for an un-64 known model by applying data constraints along with a model norm bound that differed from the 65 one used by Backus (1970a). More recently, Al-Attar (2021) has placed the method of Backus 66 (1970a) and Parker (1977) in a more general mathematical framework. 67

The second branch has mainly been represented by the SOLA method (Subtractive Optimally Localized Averages), developed by Pijpers & Thompson (1992, 1994), although similar methods had previously been used in deconvolution theory (Oldenburg 1981). The SOLA branch was introduced into the seismic tomography community by Zaroli (2016) and has received increasing attention in the past decade (e.g. Zaroli et al. 2017; Lau & Romanowicz 2021; Latallerie et al. 2022; Amiri et al. 2023; Restelli et al. 2024). Fundamentally, SOLA resembles the method by Backus (1970a), with the distinction that it lacks any prior model information such as the model

norm bound used in the DLI branch. In the absence of additional prior constraints, it yields only an 75 approximate local average - precisely defined by a resolving kernel R. Given an unknown model 76  $\bar{m}$ , the Backus (1970a) method finds a set of possible values for  $\int T\bar{m}$  (the desired property), 77 where T represents a predefined weight function, known as the target kernel. In contrast, SOLA 78 provides a single value,  $\int R\bar{m}$  (the approximate property), under error-free conditions, where R 79 is similar to T. Consequently, results obtained with approaches from the DLI branch can be in-80 terpreted in terms of the target kernels, whereas results from the SOLA branch are interpreted 81 through the resolving kernels (see Table A1). 82

The primary advantage of linear inference methods over inversions lies in their ability to pro-83 vide detailed uncertainty and resolution analyses. However, this benefit comes at the cost of lin-84 earity; these methods are only applicable to linear problems or weakly non-linear ones through 85 linearisation. While Snieder (1991) extended the method of Backus & Gilbert (1970) to address 86 weakly non-linear problems, the SOLA and DLI branches lack such generalisations. Furthermore, 87 compared to other linear methods, linear inference techniques are not ideal candidates for itera-88 tive solvers, as they focus on extracting properties of the model rather than constructing models 89 (though, as we will show later, it is possible to build discretised models as well). In non-linear 90 problems, typically a non-linear method (such as Bayesian inversion) or an iterative solver is used 91 to arrive at a model that is considered relatively close to the true model. The employed methods 92 must have convergent properties, but they do not necessarily have the ability to provide resolu-93 tion and uncertainty information. Linear inferences could then be used as a final step to provide 94 comprehensive uncertainty and resolution analysis. 95

<sup>96</sup> We propose that the combination of the two methodological branches offers a more com-<sup>97</sup> prehensive base framework for geophysical inferences. By framing the interpretation in terms of <sup>98</sup> target kernels, as is implicitly done in the DLI branch, we ensure the results are easily and consis-<sup>99</sup> tently interpretable, which is particularly important for specific applications, such as determining <sup>100</sup> relationships between seismic velocities. If the interpretation is to be placed on the target kernels, <sup>101</sup> then we argue that more care should be taken when designing the target kernels. However, the <sup>102</sup> impact of target kernel selection has not been directly studied in the SOLA branch; simple target

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kernels, such as boxcar and Gaussian functions, have typically been chosen for their ease of use
 (e.g. Zaroli et al. 2017; Restelli et al. 2024). A more careful consideration of the target kernels not
 only ensures that the advantage of easier interpretability is not lost, but it can also lead to tighter
 property bounds, as we will demonstrate.

Although the DLI branch of methods does not require the explicit use of resolving kernels, these kernels are central in the SOLA branch. We will demonstrate that, with a slight modification of the SOLA approach, the resolving kernels can also be seen as an implicit component of approaches in the DLI branch. Even within DLI methods, we can thus use these resolving kernels to obtain additional insights into spatial trade-offs and contamination from other physical parameters. In addition, if the interpretation is placed on the target kernels, it is possible to use inference methods to obtain discretised models, rather than just properties of models.

By combining the two branches, we obtain in essence a deterministic linear inference method, similar to Al-Attar (2021), but with modified property bounds and a direct incorporation of resolving kernels (an idea stemming from SOLA) into the analysis. Therefore, this combination should be regarded as a "SOLA-infused deterministic linear inference" method, which we will refer to as "SOLA-DLI".

In this contribution, we do not consider noise in the data. However, this does not mean that the 119 data are perfect. Even a noise-free dataset is not "perfect" if it lacks enough information to fully 120 constrain the model space to a single solution, i.e. it is incomplete. As Backus & Gilbert (1967a) 121 demonstrated, an infinite-dimensional model space requires an infinite number of independent 122 data to provide complete constraints. Both branches of linear inference methods discussed earlier 123 can address data noise and incompleteness, but they take fundamentally different approaches to 124 handling incompleteness. Approaches from the DLI branch integrate incompleteness errors into 125 the property bounds, while the SOLA branch captures these errors in the resolving kernels. No-126 tably, the treatment of data noise varies even within each branch (e.g., Backus (1970a) outlines 127 two distinct approaches for handling them). 128

As the two methods we aim to combine differ fundamentally in how they address incompleteness in the data, we focus in this work exclusively on errors arising from data incompleteness

rather than data noise. As a result, the framework we present is not immediately ready for most real-world applications, but it forms a foundation for future developments where data noise will be incorporated. In the mean time, the theory already has potential practical applications even without data noise considerations. For example, in design optimisation problems, where data have yet to be measured, it is the "geometry of the dataset" that drives the optimisation problem. This is exactly an element that can be addressed with the theory presented here.

The remainder of this paper is organised as follows: Section 2 firstly explores the relationship 137 between the DLI and SOLA branches, before combining them into the joint SOLA-DLI frame-138 work. In addition, we discuss the use of target and resolving kernels in SOLA-DLI, specifically, 139 showing how the choice of target kernels influences the types of properties that can be constrained 140 and how some may be better constrained than others. It further develops the theoretical frame-141 work for cases involving multiple physical parameters, explaining the roles and interpretations of 142 resolving and contaminant kernels within this context. Additionally, it demonstrates how families 143 of models can be derived using DLI-based inference methods. Section 3 presents three practical 144 examples with synthetic, noise-free data to illustrate the theoretical concepts introduced in Sec-145 tion 2. Finally, Sections 4 and 5 provide a discussion and conclusion, respectively. Appendix A 146 provides a general perspective on inference methods, while appendices B,C,D provide supplemen-147 tary mathematical derivations that offer additional detail to support Section 2. 148

#### 149 **2 THEORY**

In this section we will mathematically describe the link between the two branches of linear in-150 ferences, taking the DLI branch as starting point and subsequently introducing elements from the 151 SOLA branch to establish the SOLA-DLI framework. We also examine how the choice of target 152 kernels influences the inference outcomes and discuss key considerations necessary for ensuring 153 the correct interpretation of results. Additionally, we demonstrate how resolving kernels can be 154 employed to analyse trade-offs between physical parameters and how the model norm bound can 155 serve to estimate these trade-offs, offering a potential alternative to the 3D noise method employed 156 so far (Masters & Gubbins 2003; Restelli et al. 2024). Finally, we evaluate the strengths and lim-157

itations of linear inference methods for deriving discretised models, highlighting why "models"
 obtained with SOLA should strictly speaking be considered proxies to a model, rather than an
 actual model.

Throughout the paper, we will adopt a modern mathematical notation similar to Al-Attar (2021), which is applicable to both Banach and Hilbert spaces. This operator-based formalism is particularly well-suited for comparing and combining the SOLA and DLI methods, as it more readily clarifies the connections between these approaches.

## **2.1** Combining the DLI and SOLA branches into SOLA-DLI

#### <sup>166</sup> 2.1.1 Deterministic Linear Inferences

Let d be some error-free data, m a model, and G a linear forward operator. We can express the model-data relationship as follows:

$$G(m) = d. \tag{1}$$

We refer to such model-data relationships as "deterministic data constraints", assuming the data 169 are known exactly (no data noise). The model belongs to a model space  $\mathcal{M}$ , while the data reside 170 in a data space  $\mathcal{D}$ . In inversions, we aim to find the model solution from the data by inverting 171 the forward relation (Equation 1). However, in most cases, the forward relation cannot be inverted 172 due to insufficient or inadequate data. For continuous models, this scenario can result in either 173 no solutions or infinitely many solutions (Backus & Gilbert 1967b). In the absence of data noise, 174 no solutions occur only when the data lie outside the range of the forward operator, making them 175 incompatible with the physical laws governing the system. Typically, in such situations, we would 176 employ a different forward relation. Throughout this paper, we will assume that the data are com-177 patible with the forward relation, leading to an infinite set of solutions, denoted by S (see Fig. 1a). 178 Inversions can then be conducted by imposing constraints (regularisations) on the model space  $\mathcal{M}$ 179 until a single model,  $\tilde{m}$ , is "selected". For instance, one might choose the model with the smallest 180 average gradient (the flattest model), or with the smallest norm. However, if the implicit assump-181

tions of the chosen regularisation are incorrect, the resulting model may not accurately represent
 reality.

We often seek specific properties of the true model  $\bar{m}$  rather than the entire model itself. These properties, for example the average structure over some volume within the Earth or the depths of discontinuities, belong to a distinct space known as the property space  $\mathcal{P}$ , following the work of Al-Attar (2021). Therefore, we can define a different (inference) problem as:

Given that.

$$G(\bar{m}) = d$$
 (2)  
Find:

$$\mathcal{T}(\bar{m}) = \bar{p} \tag{3}$$

where  $\mathcal{T}$  (the property mapping) is a linear relation that extracts a property of any model, and  $\bar{p} \in \mathcal{P}$  represents the value extracted by  $\mathcal{T}$  when applied to the true model  $\bar{m}$ . It can be shown that in most practical situations, the desired property  $\bar{p}$  can take any value given a finite number of deterministic data constraints (Al-Attar 2021; Backus 1970a). In other words, given the data constraints,  $\bar{p}$  may take any value from the property space  $\mathcal{P}$  (see Fig. 1a), leaving us unable to definitively determine the property of the true model  $\bar{m}$ . Backus (1970a) demonstrated that this issue can be overcome by introducing a norm bound M in the model space:

$$\|m\|_{\mathcal{M}} \le M. \tag{4}$$

This constraint on the model space differs from constraints typically imposed during regularisation 195 because it does not aim to isolate a single model. Instead, the model norm bound restricts solutions 196 to a bounded subset of  $\mathcal{M}$ . If the set of models satisfying the norm bound is denoted by  $U_M$ 197 (Equation 4), then the set of solutions respecting both the norm bound and the data constraint 198 is  $U_M \cap S$ , which is a bounded subset (Al-Attar 2021). Al-Attar (2021) further showed that this 199 constraint results in the true property  $\bar{p}$  being confined within a bounded subset  $P \subset \mathcal{P}$ , provided 200 that the norm of the true model is less than the chosen norm bound (see Fig. 1b for a visual 201 representation of these concepts). Note that the subset P is not a sharp bound on the values of the 202

true property, meaning that  $\mathcal{T}(U_M \cap S) \subseteq P$  (theoretically, better approximations are possible). Without additional prior information, all properties in P are equally likely to represent the true property  $\bar{p}$ .

If the model space  $\mathcal{M}$ , data space  $\mathcal{D}$ , and property space P are Hilbert spaces, and the forward and property mappings  $G, \mathcal{T}$  are continuous linear mappings with G being surjective, then the solution to Equation 3 with data and model norm bound constraints (Equations 1 and 4) is given by (Al-Attar 2021):

$$\bar{p} \in \{p \in \mathcal{P} | \left\langle \mathcal{H}^{-1}(p - \tilde{p}), p - \tilde{p} \right\rangle \le M^2 - \|\tilde{m}\|_{\mathcal{M}}^2 \}$$
(5)

where  $\tilde{m}$  is the least norm solution to the data constraint (Equation 1), and  $\tilde{p} = \mathcal{T}(\tilde{m})$  is the desired property of the least norm solution. This result implies that the true property  $\bar{p}$  lies within a hyperellipsoid defined by the inequality in Equation 5. The shape of this hyperellipsoid is determined by the operator  $\mathcal{H}$ , which is given by Al-Attar (2021):

$$\mathcal{H} = \mathcal{T}\mathcal{T}^* - \mathcal{T}G^*(GG^*)^{-1}G\mathcal{T}^*.$$
(6)

It can further be shown that  $GG^*$  is invertible (Al-Attar 2021), if the model and data space are Hilbert spaces, and if G is a continuous linear and surjective mapping (we provide proof of its surjectivity in Appendix B).

#### 217 2.1.2 Considerations on the model norm bound

The true model properties lie within the property bounds only if the norm of the true model is smaller than or equal to the norm bound. Therefore, it is crucial to choose a conservative norm bound in order to minimise the risk of inferring incorrect information about the true model. Typically, we select the norm bound to be greater than the norm of the least norm solution (which we will simply refer to as the least norm from here on).

Higher norm bounds result in larger property bounds, which in turn reduces the inference power. If it is not possible to justify a sufficiently small norm bound that results in meaningful property bounds, then a least norm regularisation should not be used either. At first glance, the norm bound might appear to be a stringent constraint that is difficult to justify physically. In con-

trast, least norm regularisation, commonly used in inversion problems, simply assumes that "the true model should have a small norm". However, such regularisation essentially selects a single model, which is actually more stringent than the inequality constraint used in inference methods.

Deriving a norm bound directly from physical arguments is often challenging, but it is possible in specific cases. For example, when modeling the Earth's magnetic field using spherical harmonic coefficients, physical constraints like power dissipation can provide a norm bound. In seismology, point-wise upper bounds on properties are often more accessible. From these bounds, a model norm bound can be derived by constructing a piecewise function  $\bar{m}(x) \leq b(x)$ , leading to:

$$\int_{\Omega} \bar{m}^2 \, d\Omega \le \int_{\Omega} b^2 \, d\Omega = M^2$$

<sup>235</sup> While this approach transforms point-wise bounds into an  $L_2$  norm bound, it often overesti-<sup>236</sup> mates the bounds, resulting in overly large property bounds. A more precise alternative would be <sup>237</sup> the supremum norm:

$$\|m\|_{\infty} = \sup_{x\in\Omega} |m(x)|.$$

Alternatively, bounds based on model regularity (e.g., smoothness constraints) may be adopted, but they involve Sobolev spaces that account for derivatives. Although such approaches are more rigorous, they are mathematically complex and not fully developed, as discussed in Al-Attar (2021). Here, we use the  $L_2$  norm for simplicity as the exploration of alternative norms is beyond the scope of our work, but we acknowledge that other norms may be better suited.

#### 243 2.1.3 SOLA and resolving kernels

We can specificise the DLI inference problem to obtain the theory of Backus (1970a) by assuming the following form for the data and property mapping:

$$[G(m)]_i = \langle K_i, m \rangle_{\mathcal{M}} \tag{7}$$

$$[\mathcal{T}(m)]_k = \left\langle T^{(k)}, m \right\rangle_{\mathcal{M}},\tag{8}$$

where  $\langle \cdot, \cdot \rangle_{\mathcal{M}}$  denotes the model space inner product,  $K_i \in \mathcal{M}$  are data sensitivity kernels, and  $T^{(k)} \in \mathcal{M}$  are target kernels. Then Equations 5 and 6 correspond to the solution of Backus (1970a, Equation 4). We note that only the target kernels  $T^{(k)}$  and sensitivity kernels  $K_i$  appear in this formulation; resolving kernels are neither required nor used.

Resolving kernels do play a role in SOLA-type linear inferences, where the problem described by Equations 2 and 3 is "solved" without incorporating prior information on the model norm bound. However, the SOLA framework usually assumes an even more specific form for the data and property mapping than that shown in Equations 7 and 8, namely:

$$[G(m)]_i = \int_{\Omega} K_i m d\Omega \tag{9}$$

$$[\mathcal{T}(m)]_k = \int_{\Omega} T^{(k)} m d\Omega, \qquad (10)$$

<sup>254</sup> which corresponds to choosing the model space inner product to be

$$\langle f,g \rangle_{\mathcal{M}} = \int_{\Omega} fg d\Omega$$

and the model space to be some corresponding function space, such as  $L^2[\Omega]$ , where  $\Omega$  is some spatial domain. This choice of inner product, which is normally implicitly assumed in SOLA-type inference problems, has implications for the norm bound and its effectiveness. In particular, using this inner product leads to the following norm:

$$\|m\|_{\mathcal{M}} = \int_{\Omega} f^2 d\Omega.$$
(11)

The goal of SOLA is to find some real weights  $x_i^{(k)}$  such that (Zaroli 2019):

$$\int_{\Omega} T^{(k)} \bar{m} d\Omega \approx \int_{\Omega} \sum_{i}^{N_d} x_i^{(k)} K_i \bar{m} d\Omega$$
(12)

where  $N_d$  is the number of sensitivity kernels and the dimension of the data space  $\mathcal{D} = \mathbb{R}^{N_d}$ . The resolving kernels are then defined to be:

$$R^{(k)} = \sum_{i}^{N_d} x_i^{(k)} K_i$$
(13)

<sup>262</sup> The resulting SOLA solution is given by:

$$argmin_{x_i^{(k)}} \left[ \int_{\Omega} (T^{(k)} - \sum_i^{N_d} x_i^{(k)} K_i)^2 d\Omega \right]$$
(14)

s.t. 
$$\int_{\Omega} R^{(k)} d\Omega = 1$$
(15)

This constrained optimisation problem will provide the weights that will produce unimodular resolving kernels similar to the target kernels. Subsequently, the true properties can be approximated by:

$$[\mathcal{T}(\bar{m})]_k \approx [\mathcal{R}(\bar{m})]_k = \int_{\Omega} R^{(k)} \bar{m} d\Omega.$$
(16)

<sup>266</sup> If we drop the unimodularity condition (Equation 15), then it can be shown (Appendix C) that the <sup>267</sup> solution to the optimisation problem in Equation 14 is the same as the solution to:

$$\int_{\Omega} T^{(k)} K_j d\Omega - \sum_{i}^{N_d} \left( \int_{\Omega} K_j K_i d\Omega \right) x_i^{(k)} = 0.$$
(17)

<sup>268</sup> It is obvious from Equation 9-10 that:

$$\int_{\Omega} T^{(k)} K_j d\Omega = [\mathcal{T}G^*]_{kj}$$
(18)

$$\int_{\Omega} K_j K_i d\Omega = [GG^*]_{ji} \tag{19}$$

269 If we further define  $X_{ki} = x_i^{(k)}$ , then we find:

$$X = \mathcal{T}G^*(GG^*)^{-1}.$$
 (20)

Therefore,  $X : \mathcal{D} \to \mathcal{P}$  is a linear mapping that maps from the data space to the property space. In the absence of the unimodularity condition (Equation 15), X(d) will be the solution in the SOLA framework, obtained here without the need for a model norm bound. It is also obvious that:

$$\mathcal{R} = XG = \mathcal{T}G^*(GG^*)^{-1}G \tag{21}$$

This is the same operator that can be recognised within the definition of  $\mathcal{H}$  in Equation 6. This shows that resolving kernels are implicitly present in the solution of the norm-bound (DLI) branch of inference methods. In fact, we have the relation:

$$\mathcal{H} = (\mathcal{T} - \mathcal{R})(\mathcal{T} - \mathcal{R})^*, \tag{22}$$

which shows that the matrix  $\mathcal{H}$  encodes the difference between resolving kernels and target kernels. This difference arises due to data incompleteness and can only be quantified in the property space when norm prior bounds on the model space are incorporated.

#### 279 2.1.4 The combined SOLA-DLI framework

After establishing the link between the DLI and SOLA branches, combining the two primarily involves a practical step. This step entails calculating both the property bounds (using Equation 5) and the resolving kernels (using Equation 20), and interpreting the final result using both.

In addition, we also introduce a small modification to Equation 5. It can be shown that if Equation 5 holds, the following is also true (see Appendix D3):

$$\bar{p}^{(k)} \in \left[\tilde{p}^{(k)} - \epsilon^{(k)}, \tilde{p}^{(k)} + \epsilon^{(k)}\right],$$
(23)

285 where

$$\epsilon^{(k)} = \sqrt{\left(M^2 - \|\tilde{m}\|_{\mathcal{M}}^2\right)\mathcal{H}_{kk}}.$$
(24)

$$\tilde{p} = \mathcal{T}(\tilde{m}) = \mathcal{R}(\bar{m}) \tag{25}$$

Equation 23 represents a hyperparallelepiped in  $\mathcal{P}$  that encloses the hyperellipsoid defined by 286 Equation 5. This provides more conservative error bounds. The rationale for this modification is 287 twofold. Firstly, Equation (5) requires the computation of the full matrix  $\mathcal{H}$  and solving a system 288 of linear equations involving  $\mathcal{H}^{-1}$ . In contrast, Equation 23 only needs the diagonal terms of 289  $\mathcal{H}$ , thus decreasing the computational cost significantly. Secondly, while Equation 5 incorporates 290 information about the trade-offs between error bounds of different properties, this information is 291 often difficult to visualise and interpret in practice. Conversely, Equation 23 can be easily plotted 292 (visual explanation as to why this is the case is given in Fig. A2), making it more practical for 293 applications. 294

<sup>295</sup> Historically, the DLI branch has been applied primarily to models involving a single phys-<sup>296</sup> ical parameter, whereas the SOLA approach has also been employed for cases where the data <sup>297</sup> depend on multiple physical parameters simultaneously (e.g. Masters & Gubbins 2003; Restelli <sup>298</sup> et al. 2024). This historical distinction may partly explain why resolving kernels have traditionally <sup>299</sup> not been used in the DLI branch, as their utility becomes more significant when dealing with mul-<sup>300</sup> tiple physical parameters. We will further explore the increased significance of resolving kernels <sup>301</sup> in the context of multiple physical parameters in Section 2.3, where we discuss the concept of

contaminant kernels. However, given the importance of the target kernels, we first revisit these in
 the next section.

#### **304** 2.2 Choice of Target Kernels

Different information about the unknown model can be extracted by choosing appropriate target kernels, which need to be carefully designed if we interpret the results through them. To illustrate this, we introduce a simplified setup, where we assume the model to be a triplet of piece-wise continuous and bounded functions  $m = (m^1, m^2, m^3)$  defined on the interval [0, 1]. This leads to a 1D inference problem, however, the results can be easily generalised. The true model is assumed to be known and is plotted in Fig. 2. This model is arbitrary and has no physical significance.

#### 311 2.2.1 Local Average Targets

Previous studies have primarily used the box car function as a target kernel for its simplicity and
ease of interpretation - it gives a uniform local average (Restelli et al. 2024; Masters & Gubbins
2003). However, many other types of target kernels could be used to obtain local averages. Here,
we introduce three different averaging target kernels:

Uniform Local Average (for reference):

$$T_U^{(k)}(r) := \begin{cases} C & r \in V_k \\ 0 & \text{else} \end{cases}$$
(26)

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#### Gaussian Local Average:

$$T_{G}^{(k)}(r) := C \exp\left[-\frac{\|r - r^{k}\|_{2}^{2}}{2\sigma^{2}}\right] \quad r \in \Omega$$
(27)



(a) No norm bound applied on the model space.



(**b**) With a norm bound applied on the model space.

**Figure 1.** Schematic of general linear inference problems, illustrating the effect of bounding the model space (see Table A1 for symbol definitions). Sets with thin lines for margins represent unbounded sets, while sets with double line margins represent bounded sets. The true model is denoted by  $\overline{m}$  and the least norm model solution is denoted by  $\overline{m}$ . a) When no bounds are imposed, the property of a model that respects the data constraint may take any value in the property space, which is an unbounded set (see A1-Attar 2021, Theorem 2.2). In other words,  $\mathcal{T}(S) = P = \mathcal{P}$ . b) Applying the norm bound on the model space leads to the intersection between S and  $U_M$  to be bounded, which gets mapped under  $\mathcal{T}$  to a bounded subset of  $\mathcal{P}$ . We thus have the following relation:  $\mathcal{T}(U_M \cap S) \subseteq P \subset \mathcal{P}$ .



Figure 2. An arbitrary synthetic "true model".  $m^{j}$  denotes the physical parameters of the model.

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Bump Function Average:

$$T_B^{(k)}(r) := \begin{cases} C \exp\left[\frac{w^2}{2(r-r^{(k)})^2 - w^2}\right] & r \in V_k \\ 0 & \text{else} \end{cases}$$
(28)

318 where

$$V_k = \left[ r^{(k)} - \frac{w}{2}, r^{(k)} + \frac{w}{2} \right]$$
(29)

is the compact support of the boxcar and bump function with width w,  $\sigma$  is the standard deviation of the Gaussian, and C is in each case an appropriate normalisation constant that ensures the unimodularity of each target kernel. Examples of these averaging kernels are plotted in Fig. 3. Using these target kernels we can define, for example, the following property mappings for physical



Figure 3. Examples of averaging (a) and gradient (c) target kernels and corresponding properties of model parameter  $m^1$  (b and d) obtained using these target kernels. First column: averaging and gradient target kernels with width 0.6. Second column: property values as a function of 1000 enquiry points for different local averages and gradients of the true model using target kernels with width 0.1. The grey hatched regions represent parts of the domain where the target kernels are clipped (half-width of the target kernels). The target kernels for physical parameters  $m^2$ ,  $m^3$  are 0 since we are not interested in these parameters.

<sup>323</sup> parameter  $m^1$ :

$$\bar{p}_{U/G/B}^{1,(k)} = \mathcal{T}_{U/G/B}(m) = \int_0^1 T_{U/G/B}^{1,(k)}(r) m^1(r) dr.$$
(30)

The property vector extracted by each such property mapping (uniform/Gaussian/bump) is a vector of local averages centered at a set of points  $\{r^{(k)}\}$  that we call "enquiry points". In Fig. 3 we also plot the property vectors  $\bar{p}_{U/G/B}^{1,(k)}$  for 1000 evenly spaced enquiry points (right column). The grey

hatched regions are parts of the domain where the target kernels  $T_{U/G/B}^{1,(k)}$  are clipped and therefore their associated results uninterpretable.

Each of these target kernels has advantages and disadvantages. The boxcar function (Restelli et al. 2024) is simple and has compact support, providing a clear interpretation of the resolution of these kernels. However, most sensitivity kernels used in seismology are smooth, typically giving rise to poor resolving kernels that do not resemble boxcar functions. Consequently, the property error bounds are large.

Gaussian targets are often better reconstructed and thus lead to better constrained property val-334 ues. They are, however, not defined on a compact domain and restricting a Gaussian to a compact 335 domain leads to clipping. A clipped Gaussian is no longer a Gaussian, and different centering of 336 the Gaussian leads to different clipping and therefore a "non-uniform" interpretation of the prop-337 erty values. If most of the Gaussian is located well within the bounds of the model domain, then 338 the errors introduced by clipping can be negligible, but not readily quantifiable. For such target 339 kernels we define a "width" that contains some large and arbitrary percentage of the function's 340 weight (such as 90%) and pretend as if the entire weight of the function is concentrated in this 341 region. 342

Bump functions are both smooth and defined on a compact support, therefore offering some of the advantages of both boxcars and Gaussian targets. The one shown here is just one example of a family of functions with similar characteristics.

#### 346 2.2.2 Local Gradient Targets

<sup>347</sup> If we want to obtain some local estimate of the gradient of a 1D physical parameter such as:

$$\bar{p}^{l,(k)} = \int_0^1 T^{l,(k)} \frac{\mathrm{d}m^l}{\mathrm{d}r} dr$$
(31)

<sup>348</sup> we can use integration by parts to obtain:

$$\bar{p}^{l,(k)} = -\int_0^1 \frac{\mathrm{d}T^{l,(k)}}{\mathrm{d}r} m^l dr + \left[T^{l,(k)}m^l\right]_0^1.$$
(32)

For target kernels  $T^{l,(k)}$  with compact support Equation 32 will reduce to:

$$\bar{p}^{l,(k)} = -\int_0^1 \frac{\mathrm{d}T^{l,(k)}}{\mathrm{d}r} m^l dr$$
(33)

in the interval where the target kernels are not clipped. For any other target kernel, the second term
will not necessarily be 0. However, it will be very close to zero if the target kernel is centered well
within the bounds of the domain. Therefore, we can use Equation 33 to define new target kernels
that extract local gradients of the true model.

In the bottom row of Fig. 3 we plot the derivative of a Gaussian, Bump, and a Triangular function. The derivative of a Boxcar gives a sum of Dirac delta distributions. These cannot be used in our framework as they do not belong to a useful Hilbert space. Instead, we have opted for the derivative of a triangular function, which yields a Haar function. It is clear from Fig. 3d that the true property values obtained using the different gradient target kernels pick out the discontinuities of the true model.

The idea of using different target kernels to extract different types of information about the 360 unknown model has been applied previously in helioseismology by Pijpers & Thompson (1994). 361 They used Gaussian target kernels for extracting average information, and derivatives of the Gaus-362 sian to extract first and higher order derivatives of the model. However, as far as we are aware, 363 this approach has not yet been used in seismic tomography. More importantly, the work of Pi-364 jpers & Thompson (1994) regard this approach as an inversion, whereas we believe it should be 365 considered as an inference problem instead. While Lau & Romanowicz (2021) investigated dis-366 continuities inside the Earth using a SOLA approach, they used scalar value targets for the change 367 across discontinuity and half-Gaussian target kernels to determine volumetric trade-offs. 368

#### **369** 2.3 Resolving and Contaminant Kernels

In seismology, we often analyse data that depend on multiple physical parameters, e.g. compressional wave speed  $(v_p)$ , shear wave speed  $(v_s)$ , and density  $(\rho)$ . In general, this dependence can be expressed as:

$$[G(m)]_i = \sum_{j=1}^{N_m} \int_{\Omega} K_i^j m^j \, d\Omega, \tag{34}$$

where  $N_m$  represents the number of physical parameters. The property mapping can then be described by:

$$[\mathcal{T}(m)]_k = \sum_{j=1}^{N_m} \int_{\Omega} T^{j,(k)} m^j \, d\Omega.$$
(35)

If we consider each physical parameter as residing in its own Hilbert space  $(m^j \in \mathcal{M}_j)$ , the model space can be defined as the direct sum of these individual spaces. Consequently, a model is represented as a tuple:

$$m = (m^1, m^2, \dots, m^{N_m}).$$
 (36)

Furthermore, a norm bound for this composite model space can be derived from independent norm bounds applied to each physical parameter. This is given by:

$$\|m\|_{\mathcal{M}} = \sum_{j}^{N_m} \|m^j\|_{\mathcal{M}_j}.$$
(37)

The solution for the property bounds is then provided by Equation 5, while the corresponding resolving kernels are expressed as:

$$R^{j,(k)} = \sum_{i}^{N_d} x_i^{(k)} K_i^j.$$
(38)

It is important to note that every target kernel has an associated resolving kernel. When we are 382 interested in a specific property of the *l*-th physical parameter, we typically set all the target kernels 383 associated with other physical parameters to zero. Ideally, their associated resolving kernels would 384 then also be zero or close to zero. However, in practice, these resolving kernels are rarely zero. 385 This discrepancy increases the property bounds, making it more difficult to constrain the desired 386 property. This issue effectively highlights the trade-offs that exist between physical parameters, 387 thus providing useful information when interpreting the results. Notably, if a property of the l-th 388 parameter strongly trades off with the l'-th parameter, this will be visible in the l'-th resolving 389 kernel. 390

Any resolving kernel that is non-zero when it should ideally be zero is referred to as a contaminant kernel. Lau & Romanowicz (2021) used such contaminant kernels to quantify errors arising from trade-offs within a SOLA context. By using the model norm bound in our SOLA-DLI ap<sup>394</sup> proach, we effectively and automatically account for these trade-offs, as they are integrated into
 <sup>395</sup> the property bounds.

### **2.4** Obtaining Discretised Models through Target Kernels

One perceivable downside of linear inferences, such as SOLA-DLI, is the seeming impossibility of obtaining models that cover the full spatial domain (Valentine & Sambridge 2023). We illustrate here how SOLA-DLI can in fact be used to obtain discretised models by choosing appropriate target kernels, and discuss some advantages compared to simpler, classic inversions.

401 Consider a model  $m \in \mathcal{M}$  related to some data  $d \in \mathcal{D}$  by:

$$d_i = [G(m)]_i = \langle K_i, m \rangle_{\mathcal{M}} \,. \tag{39}$$

A common method to remove non-uniqueness, besides regularisation, is discretisation. Typically, a set of orthonormal basis functions  $\{B_l\} \in \mathcal{M}$  is chosen and any model in  $\mathcal{M}$  is projected on the subspace formed by the span of this set, leading to a parallel  $m^{\parallel}$  and perpendicular  $m^{\perp}$  component of the model (i.e.  $m^{\parallel}$  is the component that can be expressed with  $\{B_l\}$  and  $m^{\perp}$  is the residual term):

$$m = m^{\parallel} + m^{\perp} \tag{40}$$

$$m^{\parallel} = \sum_{l} p_{l} B_{l} \rightarrow \text{projection}$$
 (41)

$$m^{\perp} = m - m^{\parallel} \tag{42}$$

where  $p_l$  are the coefficients given by the projection of m onto the basis functions:

$$p_l = \langle B_l, m \rangle_{\mathcal{M}} \tag{43}$$

<sup>408</sup> We can then reformulate the initial inverse problem as:

Find 
$$\{p_l\}$$
 s.t.  
 $G\left(\sum_l p_l B_l\right) = d_i - G(\bar{m}^{\perp})$ 
(44)

The data correction term  $G(\bar{m}^{\perp})$  subtracts from the original data the component corresponding to the part of the true model that is not within the span of the basis functions. In real applications, this

term can never be computed since we do not know the true model  $\bar{m}$ , nor how much of it is outside the span of  $\{B_l\}$ . This term is therefore typically omitted and the equation solved in practice is just given by:

$$G\left(\sum_{l} p_l B_l\right) = d_i \tag{45}$$

which, combined with Equation 39, leads to the discretised inverse problem:

$$d_i = \sum_l \left\langle K_i, B_l \right\rangle p_l \tag{46}$$

In the seismic tomography literature, the matrix  $\langle K_i, B_l \rangle$  is often denoted by G. However, we will not use that notation here since we already have a distinct (but related) use of the letter G.

When the number of coefficients  $p_l$  is chosen to be smaller than the number of data, such that 417 Equation 46 is overdetermined, it is often solved in a least square (or regularised least square) 418 manner to produce the coefficients  $\{\hat{p}_l\}$ . These are systematically different from the true coeffi-419 cients  $\{\bar{p}_l\}$ , because the correction term  $G(\bar{m}^{\perp})$  is ignored. Including more data while keeping the 420 same basis functions  $\{B_l\}$  will not eliminate the systematic error caused by omitting the correc-421 tion term. In order to converge to the true solution  $\{\bar{p}_l\}$ , one has to increase both the number of 422 data and the number of basis functions in the expansion. Increasing the number of basis functions 423 shrinks the space in which  $\bar{m}^{\perp}$  resides and thus decreases the size of the correction term  $G(\bar{m}^{\perp})$ . 424 Some methods exist to mitigate or eliminate the systematic error introduced by ignoring the data 425 correction. Trampert & Snieder (1996), for example, refer to the effect of the uncorrected data as 426 leakage, and offer a method of suppressing it based on soft priors. A different method of overcom-427 ing this issue is using quadratic bounds on the model space (Backus 1988a), which we will discuss 428 in the SOLA-DLI framework. 429

The inverse problem discussed above (Equation 46) can be turned into an inference problem by defining the property mapping as:

$$[\mathcal{T}(m)]_l = \langle B_l, m \rangle_{\mathcal{M}} = p_l.$$
(47)

By also providing a model norm bound, the basis coefficients can be solved for using Equation 5. As the number of data increases, the bounds on the coefficients decrease (assuming error-free data), and the mid value of these bounds approaches the true property. This contrasts with the

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<sup>435</sup> behavior of a simple least-norm solution that – without the addition of more basis functions –
<sup>436</sup> will converge towards a systematically incorrect answer. Therefore, framing the problem as an
<sup>437</sup> inference problem, and using norm bounds, we can avoid the "leakage problem". This is basically
<sup>438</sup> the same idea as that of Backus (1988a) since a norm bound is just a specific case of a quadratic
<sup>439</sup> prior.

This approach and other similar ones have previously been explored by several authors (e.g. Al-Attar 2021; Parker 1977), especially in the context of geomagnetic modelling problems (e.g. Backus 1988a, 1989). However, these studies used mostly spherical harmonics expansions of the model. In the spirit of Section 2.2, we note that the choice of target kernels (implicitly the basis function expansion in this case) has an impact on the size of the property bounds (here the expansion coefficients), which mirrors the idea that not all basis function expansions are created equal, some of them being naturally better constrained by the data geometry than others.

Once the property bounds have been found, they can be sampled and mapped back to the model space using the adjoint of the property mapping, thereby producing actual models. Since this method generates a family of models rather than a single model, it is unclear which particular model should be selected if one intends to run an iterative inversion based on this method.

#### 451 3 APPLICATIONS

We use three case studies to showcase the advantages and capabilities of the SOLA-DLI method introduced in the previous Section. In Case 1 (Subsection 3.1), we show the effect of the prior model norm bound and choice of target kernels on the solution, illustrating how different types of properties can be constrained. In Case 2 (Subsection 3.2), we illustrate SOLA-DLI can be utilised to perform a simple resolution and trade-off analysis, even without data errors. Finally, in Case 3 (Subsection 3.3), we demonstrate how discretised model solutions can be obtained using SOLA-DLI, comparing the results with a least-squares inversion solution.



True Physical Parameters and Upper Bounds

Figure 4. Case 1: True model and model norm bounds. Panels a-c show the synthetic quasi-randomly generated true model (comprised of three physical parameters) and some arbitrary piece-wise upper bound functions  $(b_i)$  used for computing the norm bound. In each panel, we present both the physical parameter (black), and the absolute value of the physical parameter (blue).

#### 3.1 **Case 1: Effect of Different Target Kernels** 459

In this completely synthetic case study, we show how the choice of target kernels influences the 460 inference results. We also illustrate how the prior information and the desired resolution change 461 the local property estimates. 462

#### 3.1.1 Setup 463

We consider a 1D model space containing three physical parameters  $m^1, m^2, m^3$ , all of which are 464 piece-wise continuous functions defined on the interval [0, 1]. The synthetic true model (Fig. 4) is 465 generated quasi-randomly and has no physical meaning. 466



Figure 5. Case 1: Sensitivity kernels. Panels a–c show the synthetic quasi-randomly generated sensitivity kernels for physical parameters  $m^1, m^2, m^3$ . The region with no sensitivity to  $m^2$  is shaded in gray.

The model-data relationship for  $d_i$  with  $i \in \{1, 2, ..., N\}$  is given by:

$$d_{i} = [G(m^{1}, m^{2}, m^{3})]_{i} = \int_{0}^{1} K_{i}^{1}(r)m^{1}(r)dr + \int_{0}^{1} K_{i}^{2}(r)m^{2}(r)dr + \int_{0}^{1} K_{i}^{3}(r)m^{3}(r)dr$$

$$(48)$$

<sup>468</sup> For each physical parameter, the sensitivity kernels are produced quasi-randomly using the equa-<sup>469</sup> tion:

$$K_i^j(r) = \frac{1}{\sigma\sqrt{2\pi}} \exp\left(-\frac{(r-\mu_{i,j})^2}{2\sigma^2}\right) \sin(\omega r) \sum_q c_q (r-r_q)^2 \tag{49}$$

where  $\mu_{i,j}, c_q, r_q, \omega$  are randomly generated (see Fig. 5). We choose to use N = 150 (e.g. 150 observations) with the sensitivity kernels computed for each physical parameter. To simulate the lack of data sensitivity to a particular region (e.g. no S-wave sensitivity in the Earth's outer core), we manually set the sensitivity kernels for  $m^2$  to zero in the interval [0.5, 0.75]. The synthetic

<sup>474</sup> (error-free) data are then produced using Equation 48 combined with the synthetic sensitivity
<sup>475</sup> kernels and the synthetic true model. As target kernels we use those defined in Equations 26, 27
<sup>476</sup> and 28 choosing a width of 0.2.

The least norm solution to this problem (Equation 48) is given by the Moore-Penrose rightinverse:

$$\tilde{m} = G^* (GG^*)^{-1} d \tag{50}$$

and shown in Fig. 6. This is a regularised inverse solution obtained by selecting the solution with the least norm from the set of all possible solutions. We note that in this case the least norm solution approximates the true model reasonably well, except in the regions with no sensitivity (where the solution is set equal to zero), indicating that the true model norm is very close to the least norm.

To solve the SOLA-DLI inference problem, upper bound functions  $b^i$  are chosen arbitrarily (Fig. 4) such that:

$$\left| m^{j}(r) \right| \le b^{j}(r) \quad \forall r \in [0, 1],$$
(51)

<sup>485</sup> which leads to the following upper bound on the model norm:

$$\|m^{j}\|_{\mathcal{M}^{j}} = \sqrt{\int_{0}^{1} (m^{j})^{2} dr} \le \sqrt{\int_{0}^{1} (b^{j})^{2} dr} = M^{j}$$
(52)

$$||m||_{\mathcal{M}} \le M = M^1 + M^2 + M^3 \tag{53}$$

In real applications, the upper bound functions  $b^j$  should be chosen carefully based on physical arguments, for example using constraints from mineral physics, as discussed already in Section 2.1.2.

#### 489 3.1.2 Local Averages and Gradients

As introduced in Section 2.2, we consider three types of local averages (uniform local averages, Gaussian averages, and bump averages) and three types of locally averaged gradients (triangular averaged gradients, bump averaged gradients, and Gaussian averaged gradients). In this case study, we are specifically interested in obtaining these properties for parameter  $m^2$  given its region of no



Figure 6. Case 1: Least norm solution for  $(m^1, m^2, m^3)$  obtained using Equation 48.

sensitivity. We evaluate the properties at 100 equally spaced inquiry points in the spatial domain,
with the results plotted in Fig. 7 and Fig. 8.

For each type of property, at each of the 100 enquiry points, the solution (Equation 23) provides both an upper and a lower bound. Figure 7 shows that the uniform local average is the least constrained property, while the Gaussian average is the best constrained. This result is not surprising, given that the sensitivity kernels are Gaussians modulated by polynomial and sinusoidal functions. If the sensitivity kernels were more similar to boxcar functions, we should expect the uniform local averages to be better constrained.

Regions with no sensitivity are poorly constrained, as here the only constraint comes from the model norm bound. While it is unsurprising that some properties are better constrained than others, it is particularly notable that the property bounds for the local averages are so large that they provide little information about the true property values, even in regions with data sensitivity.



Property Bounds and Resolving Kernels Examples

Figure 7. Case 1: SOLA-DLI solutions for three different types of local average properties. First column: solution bounds for three types of local averages of physical parameter  $m^2$  evaluated at 100 evenly spaced enquiry points. Second column: target and resolving kernels for each type of property at the enquiry point located at  $r^k = 0.3$  with width 0.2. The approximate property represents the SOLA solution in the absence of the unimodularity condition, which is mathematically just the true model mapped through the approximate mapping  $\mathcal{R}$ .

Conversely, the Gaussian averages yield such tight bounds that we can be highly confident in the actual property values, assuming that the prior information is correct. These distinct differences in the ability to constrain the property are significant, as we are often interested in extracting meaningful information about the true model, rather than obtaining a specific type of average. Thus, it is important to recognize that the choice of averaging type can significantly impact how much information is obtained.

512

When we aim to obtain locally averaged gradients as properties, smoother target kernels again



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Property Bounds and Resolving Kernels Examples

**Figure 8.** Case 1: SOLA-DLI solutions for three different types of local averaged gradient properties, similar to Fig. 7.

lead to significantly better property bounds (Fig. 8), similar as noted for local averages. Notice
however, that while the resolving kernels look similar, the property bounds of the gradients are
typically larger than for the averages (compare Fig. 7 and Fig. 8).

In the absence of unimodularity conditions, the SOLA solution ("approximate property") is obtained by mapping the true model through the approximate mapping  $\mathcal{R}$ . Because the true model is close to the least norm model, a comparison between the true and approximate property values will give the false impression that it outperforms the DLI method. However, we must remember that approximate property values do not provide us the desired information about the true property values. In addition, the approximate property values must be interpreted through the resolving kernels, which can be rather different from the target kernels, and also vary in shape from one

enquiry point to another. Furthermore, we believe that the SOLA method also benefits from better
 designed target kernels, as they can lead to better resolving kernels and an easier interpretation of
 the results.

#### 526 3.1.3 Effect of the prior model norm bound

When we change the norm bound prior information, only the property error bounds are affected 527 (see Equation 24). This is illustrated in Fig. 9, where we show results for three different upper 528 bounds on the true model. Bound 3 is the most conservative, assuming a constant function three 529 times larger than the maximum of the true physical parameter. Bounds 1 and 2 are tighter and 530 therefore assume more prior knowledge. The bottom panel of the same figure illustrates that, 531 as expected, tighter norm bounds lead to tighter property bounds. In all cases, the range remains 532 centered on the approximate property. It is interesting to note that restricting the bounding function 533  $b^{j}$  in some local region does not lead to a tighter property bounds at an enquiry point in the same 534 region, but rather it will lead to a uniform decrease of the property bounds at all enquiry points. 535

#### 536 3.1.4 Effect of target kernel width

<sup>537</sup> Changing the width of the target kernels can be interpreted as changing the resolution of the <sup>538</sup> property evaluated at a given enquiry point. To investigate this, we have varied the target width <sup>539</sup> between 1% and 100% of the domain width and computed the relative error bounds for all the <sup>540</sup> enquiry points and widths. The results are plotted in Fig. 10. The relative error bound shown in the <sup>541</sup> first column is defined as:

$$e^{(k)} = \frac{\epsilon^{(k)}}{\max(\tilde{p}) - \min(\tilde{p})}$$
(54)

where  $\tilde{p}$  is the property of the least norm model solution  $\tilde{m}$ . This metric has been chosen as the absolute error  $\epsilon$  is not a good metric for determining whether a property is well constrained, while the classic relative error defined as  $\epsilon/\bar{p}$  cannot be computed without knowing the true property  $\bar{p}$ . While there is no quantitative rule for what constitutes an unacceptable high relative property error bound, we believe any relative error higher than 100% is "certainly too high", and relative errors less than 10% are "generally good".



**Figure 9.** Case 1: Effect of prior norm bound on the property bounds. a–c) indicate the levels of three different upper bounds on all three model parameters of the true model. Our choice of norm bound functions results in the following prior norm bounds ( $M^i$ ): 2.44 (Bound 1), 3.89 (Bound 2) and 4.34 (Bound 3), which are all larger than the true model norm of 0.32. d) Solutions corresponding to the three different model upper bounds, using a bump average for  $m^2$  as example. Tighter norm bounds lead to tighter constraints on the desired properties.

In general, we find that for all target kernel types the relative error bounds increase when 548 we decrease the width of the target kernel (i.e. increase resolution). In addition, regions with no 549 sensitivity always lead to large relative errors. As expected, the width of the uninterpretable regions 550 at the edge of the domain increases with larger target kernel width (decreasing resolution) as the 551 half-width of the kernel increases. Finally, in this setup, we find that particular properties, e.g. 552 Gaussian averages, are constrained better (i.e. lower relative error bounds) than uniform or bump 553 local averages, for all enquiry points and for target kernel widths (i.e. all resolutions), likely due 554 to the fact that Gaussian-like sensitivity kernels were used. 555

This case study illustrates the general notion that we typically use inference methods to answer specific questions about a true model rather than finding the entire model itself. In SOLA-DLI, these questions are encoded in our chosen target kernels, which should be carefully designed to improve the property bounds and facilitate straightforward interpretations. The differing extent to which we are able to retrieve different target kernels effectively shows that our data can answer some questions better than others.

#### 562 3.2 Case 2: Quasi Synthetic Normal Mode Application

In this quasi-synthetic case study, we illustrate how to use SOLA-DLI to conduct a simple resolution analysis without real data or model values nor any prior information, based solely on the sensitivity kernels of the data set. We also illustrate how the results of such a resolution analysis can be linked to trade-offs between physical parameters.

567 3.2.1 Setup

<sup>568</sup> We consider a model formed by the triplet  $m = (\delta \ln(v_s), \delta \ln(v_p), \delta \ln(\rho))$ , where  $v_s$  is shear-<sup>569</sup> wave speed,  $v_p$  is compressional-wave speed, and  $\rho$  is density (Fig. 11). Each physical parameter <sup>570</sup> is assumed to be a piece-wise continuous function defined over the interval  $[0, R_E]$  where  $R_E$  is <sup>571</sup> Earth's radius (approximately 6371 km). We aim to constrain Gaussian averages and gradients of <sup>572</sup> this synthetic true model using realistic normal mode sensitivity kernels (Woodhouse & Dahlen <sup>573</sup> 1978). Specifically, we select the same modes as in the SP12RTS dataset (Koelemeijer et al. 2016;



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**Figure 10.** Case 1: Relative error bounds with examples of resolving kernels compared to their target kernels. The different rows correspond to different types of target kernels, e.g. uniform local average (top), bump average (middle) and Gaussian average (bottom). In the three columns, we show (a) the relative error bounds e; (b) examples for wide target and resolving kernels, corresponding to the red squares in (a) and (c) examples for narrow target and resolving kernels, corresponding to the black squares in (a).

<sup>574</sup> Restelli et al. 2024), i.e. 143 modes with their sensitivity to  $\delta \ln(v_s)$ ,  $\delta \ln(v_p)$  and  $\delta \ln(\rho)$  concen-<sup>575</sup> trated mostly in the mantle (see Fig. 12).

#### 576 3.2.2 Resolution Analysis

<sup>577</sup> Before introducing any data or model values, we are able to perform a simple resolution analysis to <sup>578</sup> investigate where and on what spatial scale our data contain information regarding the Earth model. <sup>579</sup> While the SOLA-DLI solution itself depends on the model norm bound via M (see Equation 24), <sup>580</sup> indirectly on the data via  $\|\tilde{m}\|_{\mathcal{M}}$  (see Equation (25)), and on the relationships between the target



**Figure 11.** Case 2: Arbitrary quasi-random synthetic true model and the upper bound functions used to compute the prior upper bound norm.

- kernels and sensitivity kernels via  $\mathcal{H}$  (see Equations D.14–D.23), the resolving kernels only depend
- <sup>582</sup> on the data geometry, i.e. the data sensitivity kernels.
- The diagonal elements of the matrix  $\mathcal{H}$  can be shown to equal:

$$\mathcal{H}_{kk} = \sum_{j}^{N_m} \left\| T^{j,(k)} - A^{j,(k)} \right\|_{\mathcal{M}_j}^2$$
(55)

which essentially quantifies the cumulative difference between our target and resolving kernels. Using  $\mathcal{H}$  we can also define the resolving misfit as a more useful metric:

$$R_{k} = \frac{\sqrt{\mathcal{H}_{kk}}}{\sum_{j}^{N_{m}} \|T^{j,(k)}\|_{\mathcal{M}_{j}}} = \frac{\sqrt{\sum_{j}^{N_{m}} \|T^{j,(k)} - A^{j,(k)}\|_{\mathcal{M}_{j}}^{2}}}{\sum_{j}^{N_{m}} \|T^{j,(k)}\|_{\mathcal{M}_{j}}}$$
(56)

which is a generalisation of the "resolution misfit" defined in Restelli et al. (2024). The resolving misfit is 0 when all the resolving kernels associated with some property evaluated at  $r^{(k)}$  are equal to the corresponding target kernels. This would mean that our data contain exact information about



Figure 12. Case 2: Normal mode sensitivity kernels for a)  $\delta \ln(v_s)$ , b)  $\delta \ln(v_p)$  and c)  $\delta \ln(\rho)$ , obtained using a modified version of OBANI based on the work of Woodhouse & Dahlen (1978). The shaded region indicates the depth range of the outer core, where the sensitivity to  $v_s$  is zero.

the desired property and the property error bounds are 0. On the other hand, the resolving misfit 589 is equal to 1 when our resolving kernels are zero, which would correspond to a complete lack 590 of sensitivity of our data to the desired property. It is important to note that the computation of 591 the resolving misfit does not use the data vector d nor any prior model information, it only uses 592 the "geometry of the data set" (Latallerie et al. 2024). Fig. 13 illustrates the information that is 593 provided by the resolving misfit (left column). As indicated by a low resolving misfit (darker 594 shades of blue), our data mostly contain information in the mantle, as expected from this selection 595 of sensitivity kernels. The resolving misfit is also typically low for wide target kernels (>18%596 domain width, or more than 1000 km). Wide gradient kernels can be better recovered in the mantle, 597



Figure 13. Case 2: Resolution analysis for a Gaussian average (top) and gradient (bottom) target for  $\delta \ln(rho)$  using realistic mode sensitivity kernels. The resolving misfit (left) and kernels (middle and right) can be computed without the need for data or any prior norm bound information. The middle and right panels illustrate the target and resolving kernels for a wide and thin target, including the contaminant kernels that indicate trade-offs between physical parameters.

<sup>598</sup> while wide averaging kernels can be better recovered in the lower outer core, again indicating that <sup>599</sup> our choice of target (i.e. property) is important.

#### 600 3.2.3 Trade-offs between physical parameters

When our data are sensitive to two or more physical parameters, it may become difficult or impossible to obtain properties of a single parameter in isolation from the others. These trade-offs between physical parameters pose problems for interpretations, particularly in regions such as the lower mantle where the sensitivity of normal modes to seismic velocities and density is similar.

<sup>605</sup> Our setup with SOLA-DLI, where we explicitly set the target kernels for parameters not of <sup>606</sup> interest to zero, enables us to easily visualise and consider model parameter trade-offs. Suppose <sup>607</sup> we are interested in some local property of  $\delta \ln(\rho)$ , for example the Gaussian local average density <sup>608</sup> in the deep mantle or the density jump across the 660 discontinuity as characterised by a Gaussian

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gradient (Lau & Romanowicz 2021). If we choose low resolution (wide) target kernels (middle 609 column), we find that the resolving kernels for  $\delta \ln(\rho)$  match the target kernels well (Fig. 13). Fur-610 thermore, the resolving kernels for  $\delta \ln(v_s)$  and  $\delta \ln(v_p)$  also match their respective target kernels, 611 which are just zero. Such zero or near zero resolving kernels indicate that the trade-off between the 612 physical parameter of interest and the other physical parameters is small. However, if we choose 613 higher resolution (thin) target kernels (right column), we notice that the resolving kernels are strug-614 gling to match their respective target kernels. The resolving kernels for  $\delta \ln(v_p)$  and particularly 615  $\delta \ln(v_s)$  are far from zero, indicating significant trade-offs with the desired property of density, 616 which are regarded as *contaminants*. Such trade-offs between physical parameters are naturally 617 taken into account by SOLA-DLI and typically result in higher error bounds on the property. If 618 instead we would account for the sensitivity to  $\delta \ln(v_p)$  and  $\delta \ln(v_s)$  by scaling the sensitivity ker-619 nels, we would obtain tighter bounds, at the expense of assuming more prior information, similar 620 to the results of Restelli et al. (2024) using the "3D noise" approach in their SOLA inversions. 621

#### <sup>622</sup> 3.3 Case 3: Discretised inversions using continuous SOLA-DLI

This final case study serves to illustrate how we can obtain a family of discretised model solutions using SOLA-DLI, and how this approach compares to a typical least-squares inversion model solution.

#### 626 3.3.1 Setup

Here, we consider a model m with only one physical parameter, denoted also m (see the true model in Fig. 14 a)). Our model space  $\mathcal{M}$  is PCb[0, 1] and the data are given by:

$$d_i = \left\langle K_i, m \right\rangle_{\mathcal{M}} \tag{57}$$

where  $K_i$  are some quasi-randomly functions, generated again using Equation 49 (see Fig. 14 b)). In this setup, we choose to discretise the model using a Fourier expansion. The resulting basis

<sup>631</sup> functions are (see Fig. 14 c)):

$$B_{l}(r) = \begin{cases} 1, & l = 0\\ \sqrt{2}\sin\left(2\pi\frac{l+1}{2}r\right), & l \text{ odd} \\ \sqrt{2}\cos\left(2\pi\frac{l}{2}r\right), & l \text{ even} \end{cases}$$
(58)

and a possible model expansion with Fourier coefficients  $p_l$  is given by:

$$m(r) \approx \sum_{l} p_l B_l(r).$$
(59)

<sup>633</sup> The discretised model–data relation used for the least-squares inversion is:

$$d_i = \sum_l \langle K_i, B_l \rangle_{\mathcal{M}} p_l = \sum_l \Gamma_{il}^* p_l, \tag{60}$$

<sup>634</sup> where (see also Appendix D2):

$$\Gamma_{ij}^* = \langle K_i, B_l \rangle_{\mathcal{M}} \,. \tag{61}$$

This leads to the following least-squares solution for  $p_l$ :

$$\hat{p} = (\Gamma \Gamma^*)^{-1} \Gamma d \tag{62}$$

Using the least-squares solution  $\{\hat{p}_l\}$ , we can thus find the corresponding model solution by using the Fourier expansion:

$$\hat{m} = \sum_{l} \hat{p}_{l} B_{l}.$$
(63)

To obtain the SOLA-DLI solution, we consider the Fourier coefficients  $p_l$  to be elements of a property vector obtained from the property mapping:

$$p_l = [\mathcal{T}(m)]_l = \langle B_l, m \rangle_{\mathcal{M}} \,. \tag{64}$$

<sup>640</sup> We also introduce a prior model norm bound (see Fig. 14 a)). This leads to the following SOLA-

#### 641 DLI problem:

#### Given

$$d_i = \langle K_i, m \rangle_{\mathcal{M}} \tag{65}$$
  
Find

$$p_l = \langle B_l, m \rangle_{\mathcal{M}} \,. \tag{66}$$

<sup>642</sup> This problem is readily solved using Equation 23 to obtain upper and lower bounds for the possible <sup>643</sup> values of the Fourier coefficients:

$$\bar{p}_l \in [\tilde{p}_l - \epsilon_l, \tilde{p}_l + \epsilon_l]. \tag{67}$$

In this case  $\tilde{p}_l$  are the Fourier coefficients of the least norm solution to Equation 57, which are not to be confused with the single least-squares solution  $\hat{p}_l$ . In contrast, the property bounds obtained from SOLA-DLI (Equation 67) offer a family of solutions that can be sampled.

#### 647 3.3.2 Discretised least-squares vs. SOLA-DLI solution

<sup>648</sup> We compute both the least-squares and discretised SOLA-DLI solution using different number <sup>649</sup> of data points (50, 70 or 100), solving for 29 Fourier coefficients. SOLA-DLI initially provides <sup>650</sup> property bounds on the Fourier coefficients, and we therefore have to draw samples from these <sup>651</sup> distribution for each Fourier coefficient distribution to obtain a possible model solution, illustrated <sup>652</sup> in Fig. 15.

When using few data (Fig. 15, the least-squares inversion generally struggles to retrieve Fourier 653 coefficients close to the true ones, while the bounds of the SOLA-DLI solution always encompass 654 the true coefficients (true properties). That said, for certain Fourier coefficients and in certain 655 parts of the model, the least-squares solution does appear to approach the true property (Fourier 656 coefficients) and the true model better than the SOLA-DLI solution. Increasing the number of data 657 to 70 leads to a better least-squares solution, especially for the first 10 Fourier coefficients, and 658 tighter bounds of the SOLA-DLI solution. However, it now becomes clear that the SOLA-DLI 659 bounds offer more accurate information, always encompassing the true Fourier coefficients and 660 better resembling the true model compared to the least-squares solution. When we further increase 661



Figure 14. Case 3: Model setup and kernels. (a) True model m with the upper bound function used to compute the prior model norm bound. (b) Synthetic quasi-random sensitivity kernels. (c) Examples of four Fourier basis functions.

the number of data points to 100 (see Figs. 15 c) and f)), we note that the SOLA-DLI solution converges closely to the true Fourier coefficients and model, while the least-squares inversion systematically deviates.

In our synthetic setup, it is possible to explicitly compute the data correction term, which captures the components of the true model that are not within the span of the basis functions (see Section 2.4, Equation 2.4). When we correct the data, using our knowledge of the true model, we find that the least-squares inversion solution converges to the true Fourier coefficients, even for



**Figure 15.** Case 3: Comparison between least-squares and SOLA-DLI solution for a model discretised using Fourier basis functions. a–c) Fourier coefficients from discretised least-squares inversion and bounds of the SOLA-DLI solution using a) 50 data points, b) 70 data points and c) 100 data points. d–f) Discretised model solution from discretised least-squares and two samples from the SOLA-DLI property bounds using d) 50 data points, e) 70 data points.

few data (Fig. 16). This demonstrates the equivalence of the discretised least-squares and SOLA-DLI solutions. However, in real world applications, when the true model is unknown, this data correction term cannot be computed. Consequently, the SOLA-DLI solution should be preferred over the discretised least-squares inversion method. As mentioned before, there are other methods (e.g. Trampert & Snieder 1996) for bypassing or approximating the effect of the data correction term, which should also be preferred over a simple least norm inversion.

#### 675 4 DISCUSSION

In this contribution, we have introduced the SOLA-DLI framework, which combines the advantages of both DLI and SOLA branches of inferences. At present, we have focused on error-free data, as the fundamental distinction between the two branches lies in their treatment of uncertainties arising from incomplete data, not from how data noise is incorporated. However, for any



**Figure 16.** Case 3: Comparison between Fourier coefficients obtained using SOLA-DLI and the discretised least-squares method with an additional data correction term, using a) 50 data points, b) 70 data points and c) 100 data points. A comparison with the least-squares solutions in Fig. 15 indicates that the data correction leads to the systematic error in the Fourier coefficients.

real-world application, it is essential to address data noise. Al-Attar (2021), Parker (1977), and 680 Backus (1970a) have each proposed methods for incorporating noise into DLI-based approaches. 681 Since the SOLA-DLI framework integrates both methodologies, we can draw upon these exist-682 ing approaches and adapt them as necessary to introduce data noise into the framework. There 683 are numerous ways to achieve this, but it is not yet clear which approach would best balance 684 computational efficiency with the need to produce property bounds that are not excessively large. 685 Depending on the chosen approach, the matrix X may be affected by noise, which would alter the 686 final form of the resolving kernels. However, this does not render them unusable or uncomputable, 687 and crucially, it does not alter their interpretation. We believe that the selection of target kernels 688 also remains important, but in the presence of data noise, a particular set of target kernels A may 689 perform better than another set B, whereas in the absence of noise, set B might outperform set A. 690 This variability does not undermine the points that we make in the present contribution, which is 691 that some target kernels are more effective than others. A potential direction for future research 692 could be target optimisation, where, given a set of data, the goal is to identify those target ker-693 nels that produce the most effective constraints from a family of, for example, averaging weight 694 functions. We anticipate that the methods behind such an optimisation algorithm would need to 695 account for data noise. 696

697

We expect that the careful treatment of target kernels will become more involved when going

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to 2D or 3D cases (e.g. Zaroli 2016; Latallerie et al. 2022; Freissler et al. 2024). However, it 698 also opens up more possibilities. In higher dimensions, we can design target kernels sensitive to 699 directional gradients or local curvature using kernels that represent smoothed Laplacian operators. 700 Such target kernels would for example amplify the presence of a gap between two peaks rather 701 than smoothing the peaks into one, which could be useful for studying plumes (similar to the idea 702 of point-spread functions of Fichtner & Trampert (2011)). Another possible extension of our work 703 would be to replace the deterministic prior information with probabilistic information by placing 704 a prior measure on the model space, which can be updated using noisy data measurements and 705 propagated into the property space. Backus (1970a) already mentioned such a modification and 706 Al-Attar (2021) added to this discussion. Such a modification would lead to yet another possible 707 mechanism for dealing with data noise. 708

The introduction of prior model information via the model norm bound is of great importance 709 in the SOLA-DLI method. The model norm bound ( $L_2$  norm) chosen here is the most common due 710 to its mathematical simplicity, but as pointed out by Al-Attar (2021) and discussed in Section 2.1.2, 711 there might be better prior constraints. Other model norms may allow to place bounds on the 712 maximum point-value of the true model, or its gradients (smoothness) (Stark & Hengartner 1993). 713 Such modifications may necessitate the use of more general spaces than Hilbert spaces, which 714 adds significant theoretical complications. We refer the interested reader to Al-Attar (2021) for the 715 required theoretical modifications. 716

The computational cost of the methods presented arises from multiple sources. Computing the 717 matrices  $\Lambda$  ( $N_d \times N_d$ ) and  $\Gamma$  ( $N_p \times N_d$ ) requires at most  $N_m (N_d^2/2 + N_p N_d)$  integrations for  $N_m$ 718 model parameters, with the cost depending on the sensitivity and target kernels used. Sensitivity 719 kernels, especially in the case of finite-frequency adjoint methods, can be expensive to compute. If 720 sensitivity kernels already exist, the integration cost for SOL-DLI depends only on the number of 721 kernels and the integration scheme. Since  $\Lambda^{-1}$  is rarely computed explicitly, applying it involves 722 solving  $N_p + 1$  linear systems, similar to the cost of obtaining a SOLA or DLI solution without data 723 noise (Al-Attar 2021), and much lower than the classic Backus-Gilbert method (Backus & Gilbert 724 1970; Pijpers & Thompson 1992). For SOLA-DLI, these  $N_p + 1$  solves yield the final solution, 725

<sup>726</sup> while normal DLI requires additional computations involving  $\mathcal{H}^{-1}$  to assess the hyperellipsoid <sup>727</sup> constraints. When accounting for data noise, the cost depends on the method used to incorporate <sup>728</sup> it, which will likely be adapted from existing SOLA or DLI approaches. Thus, the total cost of <sup>729</sup> SOLA-DLI is expected to be comparable to DLI or SOLA, making it computationally attractive <sup>730</sup> for inference problems.

#### 731 5 CONCLUSION

In this contribution, we have presented the theory and possible applications of the SOLA-DLI 732 framework, which combines the Backus-Gilbert based SOLA method with Deterministic Linear 733 Inferences (DLI). To derive this framework, we have first demonstrate the links between these two 734 branches of inference methods, before showing how the combined framework is capable of provid-735 ing a more comprehensive analysis. We have particularly emphasised the distinction between in-736 terpreting results through target kernels versus resolving kernels. As a result, target kernel design is 737 significantly more important in SOLA-DLI. In addition, the framework is capable of incorporating 738 multiple physical parameters, with trade-offs captured by contaminant kernels. Furthermore, we 739 have demonstrated how discretised models can be obtained using these linear inference methods, 740 highlighting the advantages and disadvantages associated with different approaches. All of these 741 theoretical aspects are practically demonstrated through three synthetic, noise-free case studies, 742 with software provided to enable the reader to explore these further themselves. 743

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#### 758 7 DATA AVAILABILITY

The sensitivity kernels and all the codes used to produce the figures in this paper can be found at https://github.com/Adrian-Mag/SOLA\_DLI (Mag et al. 2024).

#### 761 APPENDIX A: OVERVIEW OF INFERENCE METHODS

In this apppendix, we present an informal overview of inference methods in the absence of data
 noise. We consider the most general form of an inference problem to be (see also Fig. 1b):

Given:					
$G(\bar{m}) = d$					
Find:					
$\mathcal{T}(\bar{m}) = \bar{p}$					
where					
$G:\mathcal{M}\to\mathcal{D}$					
$\mathcal{T}:\mathcal{M}\to\mathcal{P}$					

The true model  $\bar{m}$  is unknown, and we only have data constraints at our disposal to find some properties  $\bar{p}$  of that true model. In general, there are six choices we have to make before attempting to solve this problem: we must decide what  $G, \mathcal{T}, \mathcal{M}, \mathcal{D}, \mathcal{P}$  are, and whether we want to introduce prior information or not, which we will discuss below.

## <sup>768</sup> A1 Choice of $\mathcal{D}, \mathcal{P}, \mathcal{M}$ and $\mathcal{T}$

For most applications, we are only able to measure a finite number of data and we are typically 769 interested in a finite number of properties. In addition, the data and properties are usually real. 770 Therefore, in most cases there is only one option for the data space  $\mathcal{D}$  and property space  $\mathcal{P}$ : they 771 are  $\mathbb{R}^{N_d}$  and  $\mathbb{R}^{N_p}$  where  $N_d, N_p$  are the number of data, and the number of properties respectively. 772 The model space  $\mathcal{M}$  is most often a function space or a finite dimensional real vector space. 773 On a more fundamental level, we are interested in whether the space is simply a Banach space or 774 if it possesses an inner product structure, making it a Hilbert space. Some authors have proposed 775 solutions to inference problems in Banach spaces (e.g., Stark 2008; Al-Attar 2021), while most 776 others have focused on the more structured Hilbert space (e.g., Backus & Gilbert 1967b; Backus 777 1970a; Al-Attar 2021; Pijpers & Thompson 1994; Zaroli 2016), as this simplifies the mathematics. 778 The property mapping  $\mathcal{T}$  is typically chosen to be a linear functional, as most inference prob-779 lems focus on point evaluation, basis coefficients, or local averages, all of which are linear func-780 tionals. In this paper, we argue that a more careful consideration of these functionals can lead to 781 improved results in inference problems, particularly in the context of SOLA/DLI-type inference 782 problems (as discussed in Section 2.2). 783

#### 784 A2 Choice of forward mapping G

<sup>785</sup> We are now left with making the two most important decisions. Firstly, we need to decide whether <sup>786</sup> G is a linear or non-linear mapping. Most often, the forward problem is non-linear, which leads <sup>787</sup> to complicated inference problems. While there is some work on this front in the inference field <sup>788</sup> (Snieder 1991), the problem is generally too difficult to tackle analytically or requires vast compu-<sup>789</sup> tational resources. For this reason, inference problems usually assume G to be linear and bounded <sup>790</sup> (and therefore continuous when dealing with normed spaces), resulting in linear inferences.

For linear inferences, we can delve deeper into the structure of G. If  $\mathcal{M}$  is a Hilbert space, G is often defined as a vector of inner products with some known members of  $\mathcal{M}$  (commonly referred to as sensitivity kernels in seismology) (e.g. Backus 1970a). SOLA methods, for instance, specifically use the  $L_2$  inner product on the model space  $L_2[\Omega]$  with  $\Omega$  some spatial domain, leading to the well-known form of the forward operator seen in Equation (9).

<sup>796</sup> More complicated linear forward mappings can be used if we consider that data frequently <sup>797</sup> depend on multiple physical parameters, such as shear and compressional wave speeds, as well <sup>798</sup> as density. These problems can be addressed by considering  $\mathcal{M}$  as a direct sum of Hilbert spaces, <sup>799</sup> which itself forms a Hilbert space (e.g. Lau & Romanowicz 2021), and a forward mapping of the <sup>800</sup> form given in Equation 34. In this paper, we argue that under such choices, the analysis provided <sup>801</sup> by SOLA methods offers insights that are not readily accessible through DLI methods alone.

#### **A3** Without prior information

The last, and arguably the most important decision, concerns prior information. We note that the 803 choices of  $\mathcal{M}, \mathcal{D}$ , and G already encode some level of prior information. However, when referring 804 to additional prior information, we assume that these choices have already been fixed. If we decide 805 not to use any additional prior information, we would follow along the route of MOLA/SOLA 806 methods (e.g. Backus & Gilbert 1970; Oldenburg 1981; Pijpers & Thompson 1994; Zaroli 2016). 807 For these methods, it can be shown that we typically cannot directly infer  $\mathcal{T}(\bar{m}) = \bar{p}$ . Instead of 808 obtaining the properties of interest, we must settle for approximate properties  $\mathcal{R}(\bar{m})$  (see Fig. A1). 809 Given only the data values and geometry, the goal is then to construct an approximate mapping  $\mathcal{R}$ 810 such that: 811

$$\mathcal{R} = XG$$
, where  $\mathcal{R} : \mathcal{M} \to \mathcal{P}$  and  $X : \mathcal{D} \to \mathcal{P}$ .

In essence, this involves determining the  $N_d \times N_p$  elements of the X mapping. The original method of Backus and Gilbert (Backus & Gilbert 1967a, 1968b, 1967b, 1968a, 1970) proposed an approximate mapping designed to obtain the highest-resolution local averages at  $N_p$  points of the unknown model. This mapping is obtained by minimising the cost functions for each point one by one (see Fig. A1):

$$\int_{\Omega} (J^{(k)} A^{(k)})^2 d\Omega, \quad s.t. \int_{\Omega} A^{(k)} = 1$$

where  $J^{(k)}$  is a weight function with increasing weight further away from the *k*-th point where maximum resolution is desired. In contrast, for SOLA Pijpers & Thompson (1994) constructed an approximate unimodular mapping that resembles the predefined  $\mathcal{T}$  by minimizing the cost function:

$$\operatorname{Tr}[(\mathcal{T} - \mathcal{R})(\mathcal{T} - \mathcal{R})^*], \text{ subject to } \mathcal{R}(1) = 1,$$

where 1 represents the constant function on the left-hand side and the  $N_p$ -dimensional vector of 821 ones on the right-hand side. This is the most generic formulism, a more specific form is given in 822 Fig. A1. It turns out that solving the SOLA optimisation problem is computationally more efficient 823 than solving the optimisation problem needed for the original Backus-Gilbert method (Al-Attar 824 2021; Pijpers & Thompson 1992). This is due to the fact that the matrix to be inverted for SOLA 825 depends only on the sensitivity kernels, while for the Backus-Gilbert method it depends on both 826 the sensitivity kernels and the spatially dependent functions  $J^k$ , and thus needs to be inverted again 827 for each k-th point. 828

For linear inferences on a Hilbert model space, where the forward mapping is defined via projections onto sensitivity kernels, the approximate mapping  $\mathcal{R}$  is associated with resolving kernels. These resolving kernels offer valuable insights into the interpretation of the approximate properties  $\mathcal{R}(\bar{m})$ . Even if data noise is ignored, the resolving kernels will be imperfect due to data incompleteness and trade-offs between physical parameters. The shape of these resolving kernels thus provides information about data limitations and parameter trade-offs.

#### **A4** With additional prior information

If we introduce additional prior information, we have the choose between soft and hard prior information Backus (1988b). Hard priors are those where we assume that the true model must lie with 100% certainty within a subset of the model space.

The norm bound used in this paper is an example of a hard quadratic bound (see more here, Backus 1989). In this paper, we refer to linear inferences with hard prior information as DLI methods (Deterministic Linear Inferences) due to the deterministic nature of the prior information (Al-Attar 2021). However, in the literature, these kind of problems are also referred to as CIS <sup>843</sup> (Confidence Interval Sets) as the solutions are intervals in which the property is found (Backus
<sup>844</sup> 1988a).

Soft bounds can be imposed, for example, by introducing a soft prior via a regularisation term 845 that penalises some undesired feature of the model (for example, penalising large norms). Soft pri-846 ors via penalty terms may be considered "softer" from the perspective that we prefer some models 847 to be penalised more than others, based on our belief that they are less likely to be true. However, 848 in practice, an optimisation process is carried out, resulting typically in a single solution. This solu-849 tion strikes a balance between fitting the data and minimising the penalty. However, this is a single 850 solution, and the act of optimising a penalised cost function effectively collapses the model space 851 to a single point (thus solving the problem of non-uniqueness) and will reject any other model. In 852 contrast, a hard prior will immediately remove some models that are deemed unacceptable, but it 853 will usually keep many others that are deemed acceptable, without discriminating between them. 854 Therefore, a hard prior will be more inclusive and less stringent than a penalty-based soft prior. 855

<sup>856</sup> Soft prior assumptions and similar regularisations are essential in inversion methods, as they <sup>857</sup> help address non-uniqueness, which cannot be resolved without such constraints. This is why in-<sup>858</sup> ference methods like DLI tend to have lower precision – their assumptions are too weak to break <sup>859</sup> the non-uniqueness. Essentially, these methods trade precision for accuracy, as weaker assump-<sup>860</sup> tions reduce the likelihood of introducing bias into the solution.

Another way to impose a soft bound is by making the model space a probabilistic space with a measure to describe our prior knowledge. This would eliminate some sets of models that have zero probability, but it will usually keep many models, giving higher probability to some compared to others. Overall, we believe that the hard priors used in this paper are less stringent than penaltybased soft priors, but more stringent than probabilistic soft priors.

#### **APPENDIX B: SURJECTIVITY OF** G

An inverse problem requires three components: model space  $\mathcal{M}$ , data space  $\mathcal{D}$ , and a forward relation  $G : \mathcal{M} \to \mathcal{D}$ . In our case, let  $\mathcal{M} = L_2(\Omega)$ , a Hilbert space defined on a compact domain  $\Omega \subset \mathbb{R}$ , and  $\mathcal{D} = \mathbb{R}^{N_d}$  for some  $N_d \in \mathbb{N}$ . As discussed in Section 2.1.3 (Equation 9), the forward

	Original Backus- Gilbert (BG)	SOLA	Deterministic Linear Inferences (DLI)	SOLA-DLI
Q = 1 = + 1 = ==				
Solution	$\bar{p} \approx \int_{\Omega} R\bar{m}d\Omega$ where $R = \sum_{i} x_{i}K_{i}$ and $x_{i}$ minimise $\int_{\Omega} J^{2}R^{2}d\Omega$ s.t. $\int_{\Omega} Rd\Omega = 1$	$\bar{p} \approx \int_{\Omega} R\bar{m}d\Omega$ where $R = \sum_{i} x_{i}K_{i}$ and $x_{i}$ minimise $\int_{\Omega} (R - T)^{2}d\Omega$ s.t. $\int_{\Omega} Rd\Omega = 1$	$ \langle \mathcal{H}^{-1}(p-\tilde{p}), p-\tilde{p} \rangle $ $ \leq $ $ M^{2} - \ \tilde{m}\ _{\mathcal{M}}^{2} $	$\bar{p} \in \tilde{p} + [-\epsilon, +\epsilon]$ where $\epsilon = \sqrt{(M^2 - \ \tilde{m}\ _{\mathcal{M}}^2) diag(\mathcal{H})}$
Prior Infor- mation	None	None	$\ \bar{m}\  \le M$	$\ \bar{m}\  \le M$
Interpretation of Results	Resolving Kernel	Resolving Kernel	Target Kernel	Target Kernel (+ Resolving Kernels)
Contaminant Kernels Used?	No	Yes	No	Yes
Can Produce Model/Model Proxy	Model Proxy	Model Proxy	Model	Model
References	Backus & Gilbert (1967b, 1968a, 1970, 1968b)	Oldenburg         (1981);           Pijpers & Thompson           (1994);         Masters &           Gubbins         (2003);           Zaroli         (2016, 2019)	Backus (1970a,b,c); Parker (1977); Al- Attar (2021)	This contribution

Table 1: Comparison of different Backus-Gilbert based inference methods with noise-free data

Figure A1. Comparison of different Backus-Gilbert based inference methods in the literature in the case of noise-free data. Note that the original papers use A instead of R for resolving (or averaging) kernels, but we prefer the general R as we consider a range of targets.

<sup>870</sup> relation is defined as:

$$[G(m)]_i = \int_{\Omega} K_i(x)m(x)\,dx.$$
(B.1)

with  $x \in \Omega$ . To demonstrate that G is surjective, we utilise its dual G'. The dual space  $\mathcal{M}'$  consists of linear forms  $m' \in \mathcal{M}'$  defined on  $\mathcal{M}$  that map elements  $m \in \mathcal{M}$  to  $\mathbb{R}$ :

$$m':\mathcal{M}\to\mathbb{R}$$

Since  $\mathcal{M}$  is a Hilbert space, the Riesz Representation Theorem establishes an isomorphism  $\mathcal{L}_{\mathcal{M}}$ :

 $_{^{874}}$   $\mathcal{M}' \to \mathcal{M}$ . This means that for each  $m \in \mathcal{M}$ , there exists a unique  $m' \in \mathcal{M}'$  such that

$$\mathcal{L}_{\mathcal{M}}(m') = m.$$

Similarly, the dual space of the data space  $\mathcal{D}$  is  $\mathcal{D}'$  with an isomorphism  $\mathcal{L}_{\mathcal{D}} : \mathcal{D}' \to \mathcal{D}$ . If  $G: \mathcal{M} \to \mathcal{D}$ , then the dual mapping is defined by

$$d'(G(m)) = (G'(d'))(m), \forall m \in \mathcal{M}, \forall d \in \mathcal{D}$$

**Rearranging gives:** 

$$d'(d) = m'(m).$$

<sup>878</sup> We can express the relationship between the spaces as:

$$m' = \mathcal{L}_{\mathcal{M}} \circ G' \circ \mathcal{L}_{\mathcal{D}}^{-1}(d).$$

<sup>879</sup> We can define  $G^*$ , the adjoint of G, as:

$$G^* = \mathcal{L}_{\mathcal{M}} \circ G' \circ \mathcal{L}_{\mathcal{D}}^{-1}.$$
 (B.2)

<sup>880</sup> An equivalent definition states:

$$\langle G(m), d \rangle_{\mathcal{D}} = \langle m, G^*(d) \rangle_{\mathcal{M}}, \forall d \in \mathcal{D}, m \in \mathcal{M}$$
 (B.3)

where  $\langle \cdot, \cdot \rangle_{\mathcal{M}}$  denotes the inner product on  $\mathcal{M}$  and similarly  $\langle \cdot, \cdot \rangle_{\mathcal{D}}$  is the inner product on  $\mathcal{D}$ . This implies

$$G^*(d) = \sum_{i}^{N_d} d_i K_i(x)$$

where  $x \in \Omega$ . We can now prove the surjectivity of G.

*Proof.* According to Proposition 2.1 from Al-Attar (2021), G is surjective if and only if ker(G') =

 $\{0\}, \text{ where }$ 

$$\ker(G') = \{ d' \in \mathcal{D}' \mid G'(d') = 0 \}.$$

Using the relation between the dual and the adjoint of G (Equation B.2), we find that:

$$G' = \mathcal{L}_{\mathcal{M}}^{-1} G^* \mathcal{L}_{\mathcal{D}}$$

<sup>887</sup> where we have omitted the composition symbol "o". Therefore, we have to show that:

$$\ker(\mathcal{L}_{\mathcal{M}}^{-1}G^*\mathcal{L}_{\mathcal{D}}) = \{0\}.$$

We will show this by assuming the contrary and showing that it leads to a contradiction. Let us

assume that there exists a  $d' \in \mathcal{D}', d' \neq 0$  such that  $\mathcal{L}_{\mathcal{M}}^{-1}G^*\mathcal{L}_{\mathcal{D}}(d') = 0 \in \mathcal{M}'$ . We know that  $\mathcal{L}_{\mathcal{D}}$  is an isomorphism, therefore  $\mathcal{L}_{\mathcal{D}}(d') \in \mathcal{D}$  and  $\mathcal{L}_{\mathcal{D}}(d') \neq 0$ . Applying the adjoint of G, we have:

$$G^*(\mathcal{L}_{\mathcal{D}}(d')) = \sum_{i}^{N_d} [\mathcal{L}_{\mathcal{D}}(d')]_i K_i(x)$$

<sup>891</sup> However,  $\{K_i\}$  are linearly independent, therefore

$$G^*(\mathcal{L}_{\mathcal{D}}(d')) = \sum_{i}^{N_d} [\mathcal{L}_{\mathcal{D}}(d')]_i K_i(x) = 0 \in \mathcal{M} \text{ iff } \mathcal{L}_{\mathcal{D}}(d') = 0$$

which we already know is not the case. This means that  $G^*(\mathcal{L}_{\mathcal{D}}(d')) \neq 0 \in \mathcal{M}$ . Since  $\mathcal{L}_{\mathcal{M}}^{-1}$  is bijective, the non-zero element  $G^*(\mathcal{L}_{\mathcal{D}}(d'))$  gets mapped onto a non-zero element of  $\mathcal{M}'$ , which contradicts the initial assumption.  $\Box$ 

As a final note, we want to emphasise that the approximate nature of the theory does not imply that G is not surjective (as we have proven above).

#### **APPENDIX C:** X FROM SOLA

<sup>898</sup> For SOLA inferences, in the absence of unimodularity conditions, we want to solve:

$$argmin_{x_i^{(k)}} \left[ \int_{\Omega} (T^{(k)} - \sum_i^{N_d} x_i^{(k)} K_i)^2 d\Omega \right]$$
(C.1)

<sup>899</sup> Mathematically, this is a multi-objective minimisation problem, because we want to find  $x_i^{(k)}$  that <sup>900</sup> minimise concomitantly all squared differences between the targets and their corresponding aver-<sup>901</sup> aging kernels. Since we give the same importance to each target-resolving kernel error we want to <sup>902</sup> minimise, we can use the classic Pareto method. In other words, we try to minimise:

$$argmin_{x_{i}^{(k)}}\left[\sum_{k}^{N_{p}} \int_{\Omega} (T^{(k)} - \sum_{i}^{N_{d}} x_{i}^{(k)} K_{i})^{2} d\Omega\right]$$
(C.2)

In practice, the minimisation problem for each property can be solved independently for all other properties (mathematically equivalent to Equation C.2). This leads to an embarrassingly parallel algorithm (Zaroli et al. 2017).

<sup>906</sup> Using matrix calculus, the solution can readily be found. We first take the gradient of Equation

<sup>907</sup> C.2 and set it to zero:

$$\frac{\partial}{\partial x_l^{(q)}} \sum_k^{N_p} \left[ \int_{\Omega} (T^{(k)} - \sum_i^{N_d} x_i^{(k)} K_i)^2 d\Omega \right] = 0.$$
(C.3)

908 Because

$$\frac{\partial}{\partial x_l^{(q)}} \left( T^{(k)} - \sum_i^{N_d} x_i^{(k)} K_i \right)^2 = -2 \left( T^{(k)} - \sum_i^{N_d} x_i^{(k)} K_i \right) \left( \sum_j^{N_m} \frac{\partial x_j^{(k)}}{\partial x_l^{(q)}} K_j \right)$$

<sup>909</sup> Equation C.3 becomes:

$$-2\sum_{k}^{N_{p}} \int_{\Omega} (T^{(k)} - \sum_{i}^{N_{d}} x_{i}^{(k)} K_{i}) \left(\sum_{j}^{N_{m}} \frac{\partial x_{j}^{(k)}}{\partial x_{l}^{(q)}} K_{j}\right) d\Omega = 0$$
(C.4)

910 It is obviously that:

$$\frac{\partial x_j^{(k)}}{\partial x_l^{(q)}} = \delta_{lj} \delta_{qk},$$

<sup>911</sup> which can be substituted in Equation C.4 to obtain:

$$\int_{\Omega} (T^{(q)} - \sum_{i}^{N_d} x_i^{(q)} K_i) K_l d\Omega = 0.$$
 (C.5)

<sup>912</sup> Separating the integral in Equation C.5, we now get:

$$\sum_{i}^{N_d} x_i^{(q)} \int_{\Omega} K_i K_l d\Omega = \int_{\Omega} T^{(q)} K_l d\Omega.$$

<sup>913</sup> This can be written in matrix form as:

$$X\Lambda = \Gamma,$$

914 where

$$\Lambda_{il} = \int_{\Omega} K_i K_l d\Omega$$
$$\Gamma_{ql} = \int_{\Omega} T^{(q)} K_l d\Omega$$
$$X_{qi} = x_i^{(q)}.$$

915 This finally gives us:

$$X = \Gamma \Lambda^{-1} \tag{C.6}$$

<sup>916</sup> which is equivalent to the Equations 18, 19, and 20.

## 917 APPENDIX D: ELEMENTS NEEDED FOR THE DERIVATION OF THE SOLA-DLI 918 SOLUTION

<sup>919</sup> In this appendix we derive some further equations and equalities related to the material presented <sup>920</sup> in Section 2.1.

### 921 D1 Data-model relationships

Given a model  $m = (m^1, m^2, ...)$ , the relationship between the model and data is defined by:

$$d_i = [G(m)]_i = \sum_{j}^{N_m} \left\langle K_i^j, m^j \right\rangle_{\mathcal{M}_j}.$$
 (D.1)

<sup>923</sup> It is useful to define:

$$G^{j}(m) = \left\langle K_{i}^{j}, m^{j} \right\rangle_{\mathcal{M}_{j}} \tag{D.2}$$

$$G = \sum_{j}^{N_m} G^j. \tag{D.3}$$

The adjoint of G is defined in Equation B.3 and repeated for convenience:

$$\langle G(m), d' \rangle_{\mathcal{D}} = \langle m, G^*(d') \rangle_{\mathcal{M}}$$
 (D.4)

for all  $m \in \mathcal{M}$  and  $d' \in \mathcal{D}$ . We expand the LHS:

$$\sum_{i}^{N_d} \sum_{j}^{N_m} \left\langle K_i^j, m^j \right\rangle_{\mathcal{M}_j} d'_i = \left\langle m, G^*(d') \right\rangle_{\mathcal{M}}$$
(D.5)

For the RHS, we use the formula for the inner product in the direct sum space  $\mathcal{M}$ :

$$\langle a, b \rangle_{\mathcal{M}} = \sum_{j}^{N_m} \left\langle a^j, b^j \right\rangle_{\mathcal{M}_j}$$
 (D.6)

where a, b are some members of  $\mathcal{M}$ . Therefore, we write

$$\sum_{i}^{N_d} \sum_{j}^{N_m} \left\langle K_i^j, m^j \right\rangle_{\mathcal{M}_j} d'_i = \sum_{j}^{N_m} \left\langle m^j, G^{j*}(d') \right\rangle_{\mathcal{M}_j} \tag{D.7}$$

Taking the sum over i inside, we can also write:

$$\sum_{j}^{N_m} \left\langle \sum_{i}^{N_d} d'_i K^j_i, m^j \right\rangle_{\mathcal{M}_j} = \sum_{j}^{N_m} \left\langle m^j, G^{j*}(d') \right\rangle_{\mathcal{M}_j}$$
(D.8)

<sup>929</sup> and we identify:

$$G^{j*}(d') = \sum_{i}^{N_d} d'_i K^j_i$$
 (D.9)

$$G^* = (G^{1*}, G^{2*}, ...)$$
 (D.10)

 $G^*$  maps elements from the data space to elements (tuples) in the model space. A similar approach shows that the adjoint of the property mapping  $\mathcal{T}$  is given by:

$$\mathcal{T}^{j*}(p) = \sum_{k}^{N_p} p^{(k)} T^{j,(k)}$$
(D.11)

$$\mathcal{T}^* = (\mathcal{T}^{1*}, \mathcal{T}^{2*}, ...)$$
 (D.12)

#### 932 D2 H matrix

The  $\mathcal{H}$  matrix introduced in Section 2.1 quantifies the difference between the target and resolving kernels. It is defined by Al-Attar (2021, see Equation 2.84) as:

$$\mathcal{H} = HH^* \tag{D.13}$$

$$H = \mathcal{T} - \mathcal{R} \tag{D.14}$$

where  $\mathcal{R}$  is the "approximate mapping", given by:

$$\mathcal{R} = \mathcal{T}G^*(GG^*)^{-1}G \tag{D.15}$$

This mapping takes any model  $m \in \mathcal{M}$  into the data space  $d \in \mathcal{D}$ , then finds the least norm solution to G(m) = d and maps this least norm solution into the property space. When applied to one of the possible model solutions  $U_M \bigcap S$  (see Fig. 1b), it gives the property of the model solution that has the smallest norm. Combining (D.13), (D.14), and (D.15) we obtain:

$$\mathcal{H} = (\mathcal{T} - \mathcal{R})(\mathcal{T} - \mathcal{R})^* \tag{D.16}$$

$$\mathcal{H} = \mathcal{T}\mathcal{T}^* - \mathcal{T}G^*(GG^*)^{-1}G\mathcal{T}^*$$
(D.17)

940 Let us denote

$$\Lambda := GG^*. \tag{D.18}$$

<sup>941</sup> Using a simple application of Equation (D.1) and (D.10), we can then easily obtain:

$$\Lambda_{iq} = \sum_{j}^{N_m} \left\langle K_i^j, K_q^j \right\rangle_{\mathcal{M}_j} \tag{D.19}$$

<sup>942</sup> Similarly, we denote:

$$\chi := \mathcal{T}\mathcal{T}^* \tag{D.20}$$

$$\chi_{k,l} = \sum_{j}^{N_m} \left\langle T^{j,(k)}, T^{j,(l)} \right\rangle_{\mathcal{M}_j} \tag{D.21}$$

<sub>943</sub> and

$$\Gamma := \mathcal{T}G^* \tag{D.22}$$

$$\Gamma_{ki} = \sum_{j}^{N_m} \left\langle T^{j,(k)}, K_i^j \right\rangle_{\mathcal{M}_j} \tag{D.23}$$

<sup>944</sup> Using the definitions of  $\Lambda$ ,  $\chi$ ,  $\Gamma$  we can write (D.17) as:

$$\mathcal{H} = \chi - \Gamma \Lambda^{-1} \Gamma^T. \tag{D.24}$$

Figure A2 provides a visualisation of the ellipse in the property space as determined by  $\mathcal{H}$  when only two properties are considered.

#### 947 D3 Error Bounds

The error bounds defined in Equations 23 and 24 are derived from the property bounds defined by Al-Attar (2021, see Equation 2.84) as:

$$\left\langle \mathcal{H}^{-1}(p-\tilde{p}), p-\tilde{p} \right\rangle_{\mathcal{P}} \le M^2 - \left\| \tilde{m} \right\|_{\mathcal{M}}^2$$
 (D.25)

Equation (D.25) describes a hyperellipsoid centered on  $\tilde{p}$  with major axes given by the eigenvalues of  $\mathcal{H}^{-1}$  scaled by  $\sqrt{M^2 - \|\tilde{m}\|_{\mathcal{M}}^2}$ . If the matrix  $\mathcal{H}$  is diagonal, then the inverse is trivial to find and the hyperellipsoid has its major axes aligned with the coordinate axes of the property space. In all other cases, the hyperellipsoid will have some arbitrary orientation and  $\mathcal{H}$  will be difficult to invert numerically.



<sup>956</sup> error bounds given in the form:

$$\|p - \tilde{p}\|_{\mathcal{P}}^2 \le (M^2 - \|\tilde{m}\|_{\mathcal{M}}^2) diag(\mathcal{H})$$
(D.26)

where  $diag(\mathcal{H})$  is the diagonal of  $\mathcal{H}$ . We can also write this in component form:

$$\|p^{(k)} - \tilde{p}^{(k)}\|_{\mathcal{P}}^2 \le (M^2 - \|\tilde{m}\|_{\mathcal{M}}^2)\mathcal{H}_{kk}$$
 (D.27)

Inequality (D.27) describes a hyperparallelepiped that contains the error bounds of (D.25) with 958 sides parallel to the coordinate axes of  $\mathcal{P}$  (see Fig. A2). As this approximation does not require 959 the inversion of the  $\mathcal{H}$  matrix, it is computationally advantageous. Visually, the hyperellipsoid 960 fits "perfectly" inside the hyperparallelepiped (Fig. A2), but the error bounds of the hyperpar-961 allelepiped are easier to visualise in a static plot (see for example first column of Fig. 7). The 962 hyperellipsoid encodes the correlations between the error bounds of the various components of the 963 property vector (such as the correlation between the error bounds of two different local averages). 964 Plotting the bounds for each component of the property vector simultaneously would therefore be 965 very difficult, since the error bounds of each property component would depend on the values of 966 the bounds on all other property components. The hyperparallelepiped ignores these correlations, 967 simplifying thus the plotting. However, it overestimates the property bounds, which will likely 968 make it more difficult to interpret the property values. 969

#### To show how (D.27) arises from (D.25), we need to prove the following:

#### Given that

$$x^T A^{-1} x \le b$$
 (D.28)  
Show that  
 $x_k^2 \le b A_{kk}$  (D.29)

<sup>971</sup> where  $x = \tilde{p} - \epsilon$ ,  $A = \mathcal{H}$ , and  $b = M^2 - \|\tilde{m}\|_{\mathcal{M}}^2$ . To prove this, we start by finding the maxi-<sup>972</sup> mum extent of the hyperellipsoid (D.28) along the  $k^{th}$  coordinate axis, which can be described

<sup>973</sup> mathematically as:

Find 
$$\max(c^T x)$$
 (D.30)

Given that 
$$x^T A^{-1} x \le b$$
. (D.31)

where  $c^T$  will be chosen later to be a vector with all entries 0 except the  $k^{th}$  one. We shall use the Lagrangian approach to solve this problem. We introduce the slack constant *s* and use it to transform the inequality D.31 into an equality (slack constraint):

$$x^T A^{-1} x - b + s^2 = 0 (D.32)$$

Let  $\lambda$  be a Lagrange multiplier. The problem then becomes finding the extremum points of the Lagrangian:

$$f(x,\lambda) = c^T x + \lambda (b - x^T A^{-1} x - s^2).$$
 (D.33)

<sup>979</sup> Differentiating f with respect to x and setting the result to zero leads to:

$$c - 2\lambda A^{-1}x = 0. \tag{D.34}$$

Notice that  $\lambda = 0$  leads to c = 0, which is a contradiction. Therefore we must have  $\lambda \neq 0$  and  $s^2 = 0$ , which means that our constraint is active. Assuming  $A^{-1}$  to be invertible, we obtain:

$$x = \frac{Ac}{2\lambda}.$$
 (D.35)

We next differentiate f with respect to  $\lambda$  (using  $s^2 = 0$  since we have shown the constraint to be active) to obtain the second Lagrange equation. Setting the result equal to zero leads to:

$$b - x^T A^{-1} x = 0. (D.36)$$

Substituting (D.35) into (D.36) and rearranging for b, we obtain:

$$b = \left(\frac{Ac}{2\lambda}\right)^T A^{-1} \frac{Ac}{2\lambda}.$$
 (D.37)

 $_{985}$  Since A is symmetric this leads to:

$$\lambda^2 = \frac{c^T A c}{4b}.\tag{D.38}$$

Assuming that A is positive definite (its eigenvalues give the lengths of the hyperellipsoids' major

<sup>987</sup> axes), we must have

$$\lambda = \frac{\sqrt{c^T A c}}{2\sqrt{b}}.\tag{D.39}$$

Finally, using (D.38) and (D.35) the optimal vector solution x can be expressed for any vector *c* as:

$$x = \frac{Ac}{2\lambda} = \frac{Ac}{\frac{\sqrt{c^T Ac}}{\sqrt{b}}} = \frac{\sqrt{bAc}}{\sqrt{c^T Ac}},$$
(D.40)

and the maximal value of  $c^T x$  is thus:

$$\sqrt{bc^T A c}$$
. (D.41)

Now, we consider a fixed index k between 1 and N, and we define c to be the following vector:

$$c := (\delta_{ik})_{1 \le i \le N},\tag{D.42}$$

where  $\delta_{ik}$  is 1 if i = k, and 0 if  $i \neq k$ . Substituting this for c in (D.41), we obtain:

$$\max(x_k) = \sqrt{bA_{kk}} \tag{D.43}$$

<sup>993</sup> or equivalently:

$$x_k \le \sqrt{bA_{kk}} \tag{D.44}$$

<sup>994</sup> If instead we choose  $c = -\delta_{ik}$ , then we have:

$$x_k \ge -\sqrt{bA_{kk}} \tag{D.45}$$

<sup>995</sup> These two inequalities can be summarised in the final answer:

$$(x_k)^2 \le bA_{kk} \tag{D.46}$$

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**Table A1.** Table summarising the main mathematical symbols used in the manuscript. Elements are grouped on columns and rows depending on the relationships between them. For example,  $\bar{m}$  is part of the model space  $\mathcal{M}$  and is related to  $\bar{d}$  through G, which is determined by K. Similarly,  $\tilde{p}$  is related to  $\bar{m}$  through  $\mathcal{R}$ and to  $\tilde{m}$  through  $\mathcal{T}$ .

$\mathcal{M}$	$\mathcal{D}$	$\mathcal{P}$		
Model space	Data space	Property space	Mapping	Kernels
$ar{m}$ : TRUE model	$ar{d}$ : TRUE data		G: Forward mapping	K: Sensitivity kernels
$\bar{m}$ : TRUE model		$\bar{p}$ : TRUE property	$\mathcal{T}$ : Property mapping	T: Target kernels
$\bar{m}$ : TRUE model		$\tilde{p}$ : Aproximate property	R: Approximate mapping	R: Resolving kernels
<i>m</i> : Least norm model		<i>p</i> ̃: Aproximate property	$\mathcal{T}$ : Property mapping	T: Target kernels
		$\epsilon$ : Property error	H: Hyperellipsoid matrix	
<i>j</i> : Physical parameter index	<i>i</i> : Data index	k: Property index		
$N_m$ : Number of physical parameters	$N_d$ : number of data			$N_p$ : Number of properties

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Figure A2. Illustration of the relationship between the hyperellipsoid defined in Equation D.25 and the hyperparallelepiped defined in Equation D.27 for the case when the property space is two-dimensional.  $p_1$  and  $p_2$  could represent, for example, two local averages at two different spatial locations. The dark shaded ellipse contains all the possible combinations of these two properties given by the tighter inequality of Equation D.25. The lighter gray shaded rectangle contains all the possible combinations of these two properties under the simplified inequality in Equation D.27.

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